Development of hydrologic processes in the DNDC model to explore beneficial management for reducing nutrient losses from cropping systems

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Abstract

Food production using sustainable practices to maintain or increase crop yields while limiting negative anthropogenic influences on the environment is an important global research activity. Biophysical agricultural models can be effective science-based management tools for assessing sustainability providing they are frequently updated with new knowledge and are expanded to encompasses the necessary interacting environmental processes. The DeNitrification DeComposition (DNDC) model is one of the most widely used process-based models for estimating GHG emissions and soil C and N cycling yet its ability to simulate soil hydrology and water quality requires improvement before it can reliably be used to track the trade-offs between water and nutrient losses from agricultural activities. In this thesis alternative soil hydrology formulations are investigated and implemented in DNDC to enable more precise and informative explorations of agricultural management and climate impacts on cropping systems.

The performance of the default DNDC model, which utilizes simplified water processes was compared to the more hydrologically complex Root Zone Water Quality Model (RZWQM2) to determine which processes were sufficient for simulating water and nitrogen dynamics and improvements were recommended. Both models performed adequately across a wide range of metrics including crop yields, biomass, annual and monthly water and N loss to tile drains. However, RZWQM2 performed better for simulating soil water content, and the dynamics of daily water flow to tile drains (DNDC: NSE -0.32 to 0.24; RZWQM2: NSE 0.35 to 0.69), where NSE is the Nash-Sutcliffe model efficiency. DNDC overestimated soil water content near the soil surface and underestimated it in the deeper profile. We recommended that developments be carried out for DNDC to include improved root density and penetration functions, a heterogeneous and deeper soil profile, a fluctuating water table and a new tile drainage sub-model.

Based on these findings another study was performed to enhance the hydrological framework in DNDC. A new quasi-2D sub-model for tile drainage, improved water flux, root growth dynamics, and a deeper and heterogeneous soil profile was included. Comparisons were conducted against RZWQM2, using measurements of soil water storage, runoff and drainage in eastern Canada and the US Midwest. Simulation of soil water storage (DNDC $0.81 \leq d \leq 0.90$; RZWQM2 $0.76 \leq d \leq 0.84$), daily water flow (DNDC $0.76 \leq d \leq 0.88$; RZWQM2 $0.77 \leq d \leq 0.90$)

and nitrogen loading to tile drains was greatly improved post-development, where d is the Wilmott index of agreement. DNDC was able to capture the observed differences in water and N losses between conventional drainage and controlled drainage management with sub-irrigation. Thus a widely used agroecosystem model was expanded to simulate impacts of tile drainage depth and spacing, controlled drainage and sub-irrigation on crop growth and sustainability.

The validated DNDC model was then used to investigate 18 fertilizer management options to examine N losses over a multi-decadal horizon at locations in eastern Canada and the US Midwest. Management scenarios included variable formulation (organic versus inorganic), timing (spring, fall, split, side-dress) and method of application (injected, incorporated, and broadcast). Reactive N losses (NO_3^- from drainage and runoff, N_2O and NH_3) were greatest from broadcast applications, followed by incorporated and then injected. Amongst the fertilizer timing scenarios, fall manure application resulted in the greatest N loss, primarily due to increased N leaching in non-growing season periods, with 58% more N loss per ton silage than spring application. Split application mitigated losses more so than side-dress by reducing the soil pH shift due to urea hydrolysis and NH_3 volatilization during the warmer June period. This assessment helps to distinguish which fertilizer practices are more effective in reducing N loss over a long-term time horizon which could assist farmers in weighing the trade-offs between field trafficability, manure storage capacity and expected N loss.

The revised DNDC model was used to compare and evaluate modelling approaches commonly used for predicting climate change impacts on cropping systems. These included the use of a minimum set of weather variables, re-initializing soil status annually, fixed fertilizer application rates, fixed planting dates, and ignoring changes in crop cultivars and rotational impacts. Case studies were performed at three locations that varied greatly in precipitation. In comparison to our recommended approach, whereby we simulated long-term feedbacks in C&N and water over time and employed detailed climate and agronomic drivers, we found significant differences for each approach, either in crop yields, N_2O emissions, N leaching, or N runoff. We conclude that there are often large differences between approaches and we recommend that modellers improve their capabilities of simulating biophysical processes and expected changes in agronomic practices over time.

Résumé

La production alimentaire utilisant des pratiques durables pour maintenir ou augmenter les rendements agricoles tout en limitant les influences anthropiques négatives sur l'environnement est une activité de recherche mondiale importante. Les modèles biophysiques peuvent constituer des outils de gestion scientifiques efficaces pour évaluer si l'agriculture est viable, à condition qu'ils soient fréquemment mis à jour avec de nouvelles connaissances qui englobent les processus environnementaux et les interactions nécessaires. Le modèle de DeNitrification DeComposition (DNDC) est l'un des modèles le plus largement utilisés pour estimer les émissions de GES et le cycle de C & N du sol, mais sa capacité à simuler l'hydrologie du sol et la qualité de l'eau doit être améliorée avant de pouvoir être utilisée de manière fiable pour estimer les pertes en eau et en éléments nutriments des activités agricoles. Dans cette thèse, des formulations alternatives d'hydrologie des sols sont étudiées et mises en œuvre dans DNDC pour permettre des explorations plus précises et informatives de la gestion agricole et des impacts du climat sur les systèmes de culture.

Les performances du modèle DNDC, qui utilise des processus d'eau simplifiés par défaut, ont été comparées au modèle de qualité de l'eau de la zone des racines (RZWQM2), plus complexe sur le plan hydrologique, afin de déterminer les processus suffisants pour simuler la dynamique de l'eau et de l'azote et de recommander des améliorations. Les deux modèles ont donné de bons résultats sur un large groupe de paramètres, notamment le rendement des cultures, la biomasse, les pertes annuelles et mensuelles en eau et en azote dans les drains souterrains. Cependant, RZWQM2 s'est mieux performé pour simuler la teneur en eau du sol et la dynamique du débit quotidien d'eau vers les drains souterrains (DNDC: NSE -0,32 à 0,24; RZWQM2: NSE 0,35 à 0,69). Le modèle DNDC a surestimé la teneur en eau du sol près de la surface et l'a sous-estimée en profondeur. Nous avons recommandé que des développements soient entrepris pour que DNDC inclue des fonctions améliorées de la densité et de la pénétration des racines, un profil de sol hétérogène et plus profond, une nappe phréatique fluctuante et un nouveau sous-modèle de drainage souterrain.

Sur la base de ces résultats, une autre étude a été réalisée pour améliorer le cadre hydrologique de DNDC. Un nouveau sous-modèle quasi 2D pour le drainage souterrain, l'amélioration du flux d'eau, la dynamique de croissance des racines et un profil de sol plus profond et hétérogène a été inclus. Des comparaisons ont été effectuées avec RZWQM2 à l'aide

de mesures du stockage de l’eau du sol, du ruissellement et du drainage dans l’est du Canada et du Midwest américain. Simulation du stockage de l’eau du sol DNDC $0,76 \leq d \leq 0,88$; RZWQM2 $0,77 \leq d \leq 0,90$) et la charge en azote dans les drains souterrains a été grandement améliorée après le développement. Le modèle DNDC a été en mesure de saisir les différences observées dans les pertes en eau et en azote entre le drainage conventionnel et la gestion du drainage contrôlé avec irrigation sous la surface. Ainsi, un modèle d’agroécosystème largement utilisé a été amélioré pour simuler les effets, de la profondeur et de l’espacement du drainage sous la surface, du drainage contrôlé et de l’irrigation sous la surface, sur la croissance et la viabilité des cultures.

Le modèle DNDC validé a ensuite été utilisé pour étudier 18 options de gestion des engrais afin d’examiner les pertes en azote sur un horizon pluriannuel dans des régions de l’est du Canada et du Midwest américain. Les scénarios de gestion comprenaient la formulation (organique par rapport à inorganique), le moment choisi (printemps, automne, split, bandes latérales) et méthode d'application (par injection, incorporation et à la volée). Les pertes en N réactif (NO3- provenant du drainage et du ruissellement, N2O et NH3) ont été les plus importantes après à la volée, suivies de l'incorporation puis de l'injection. Parmi les scénarios d'épandage d'engrais, l'épandage d'automne de fumier a entraîné la plus grande perte d'azote, principalement en raison de la lessivage accrue de l'azote en dehors de la saison de croissance, avec une perte d'azote supérieure de 58% par tonne ensilage de maïspar rapport à l'application au printemps. L'application fractionnée a permis d'atténuer les pertes en réduisant le pH du sol en raison de l'hydrolyse de l'urée, ce qui a entraîné une volatilisation réduite de NH3 pendant la période plus chaude de juin. Cette évaluation a permis de distinguer les pratiques d'engrais les plus efficaces pour réduire les pertes d'azote sur un horizon à long terme, ce qui pourrait aider les agriculteurs à choisir entre la capacité de stockage du fumier et les pertes prévues d'azote.

Le modèle DNDC révisé a été utilisé pour comparer et évaluer les approches de modélisation couramment utilisées pour prévoir les impacts des changements climatiques sur les systèmes de culture. Celles-ci comprenaient l’utilisation d’un ensemble minimal de variables météorologiques, la réinitialisation annuelle de l’état du sol, des taux d’application d’engrais fixes, des dates de semis fixes, et l’ignorance des changements de cultivars et des effets de rotation. Des études de cas ont été effectuées à trois endroits où les précipitations variaient considérablement. En comparaison avec notre approche recommandée, qui consistait à simuler les rétroactions à long terme de C & N et de l'eau au fil du temps et à utiliser des facteurs

climatiques et agronomiques détaillés, nous avons constaté des différences significatives pour chaque approche, en termes de rendement des cultures, d'émissions de N2O, de lessivage ou de ruissellement d'azote. Nous concluons qu'il existe souvent de grandes différences entre les approches et nous recommandons aux modélisateurs d'améliorer leurs capacités de simulation des processus biophysiques et des changements attendus dans les pratiques agronomiques au fil du temps.

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Contributions of authors

The thesis was written in manuscript-based format. The process-based modelling performed in each study was of multi-disciplinary nature bridging soil science, plant science, biochemistry and hydrology. As well, several detailed datasets were needed for model evaluation thus several researchers were involved in each manuscript. For each manuscript, Ward Smith, Ph.D. candidate under the supervision of associate professor Zhiming Qi, developed the study objectives, formulated mathematical solutions to address the research, performed model simulations, analysed results and prepared the draft papers. Dr. Zhiming Qi who provided guidance and research ideas for model development and water quality data for chapters 3-5 was a co-author on chapters 3-6 (all manuscripts). Brian Grant, who was a co-author on chapters 3-6, shared scientific principles and views on model evaluation and development and assisted in implementing equations and formulations in the DNDC code. Dr. Andrew VanderZaag, who was a co-author on chapters 3-6, provided linkages and information from other research projects on water quality and shared detailed water quality datasets. Dr. Wentian He, who was co-author on chapters 4-6, provided insights into model development needs, rigorously tested our revised model, and assisted with graphical and statistical procedures. Dr. Craig Drury shared datasets which were used in chapters 4-6. Dr. Raymond Desjardins shared his experience on modelling and water balance estimates for chapter 3. Dr. Matthew Helmers shared water quality data for chapters 4 and 5. Dr. Xavier Verge, Dr. Hambaliou Balde, and Dr. Robert Gordon shared scientific viewpoints relating to fertilizer management activities under tile drained crop production for chapter 5. Dr. Budong Qian provided downscaled climate change data for chapter 6. Dr Mervin St, Luce provided cropping system data for chapter 6. All co-authors reviewed each of the respective manuscripts they were involved with.

Scientific manuscripts included in this thesis

Chapter 3**. Smith, W.**, Z. Qi, B. Grant, A. VanderZaag, and R. Desjardins. 2019. Comparing hydrological frameworks for simulating crop biomass, water and nitrogen dynamics in a tile drained soybean-corn system: Cascade vs computational approach. Journal of Hydrology X. 2: 100015. https://doi.org/10.1016/j.hydroa.2018.100015

Chapter 4. **Smith, W.**, B. Grant, Z. Qi, W. He, A. VanderZaag, C.F. Drury, and M. Helmers. 2019. Development of the DNDC model to improve soil hydrology and incorporate mechanistic tile drainage: A comparative analysis with RZWQM2. Environmental Modelling and Software. 123:104577. https://doi.org/10.1016/j.envsoft.2019.104577

Chapter 5. **Smith, W.,** B. Grant, Z. Qi, W. He, A. VanderZaag, C.F. Drury, X. Verge, H. Balde, R. Gordon, and M. Helmers. 2019. Assessing the impacts of climate variability on fertilizer management decisions for reducing nitrogen losses from corn silage production. Journal of Environmental Quality. 48(4):1006-1015. doi:10.2134/jeq2018.12.0433

Chapter 6. **Smith, W.**, B. Grant, Z. Qi, W. He, B. Qian, A. VanderZaag, C.F. Drury, and M. St Luce. 2019. Towards an approach for modelling the impacts of climate change on cropping systems. Environmental Research Letters. Under review by co-authors.

Related scientific manuscript

In the below study the revised DNDC model, which was improved for simulating soil hydrology in this thesis, was successfully evaluated for simulating N_2O emissions and N loading to tile drains at a site near Ottawa, Ontario. The site data and model validation results were used for one of three case studies modelled in Chapters 5 and 6.

He, W., **W. Smith**, B. Grant, A. VanderZaag, , E. Schwager, Z. Qi, D. Reynolds, and C. Wagner-Riddle. 2019. Understanding the Fertilizer Management Impacts on Water and Nitrogen Dynamics for a Corn Silage Tile-Drained System in Canada. J. Environ. Qual. 48(4):1016-1028. doi:10.2134/jeq2018.11.0414.

Conference and workshop presentations

Smith, W., Z. Qi, B. Grant, W. He, A. VanderZaag, C. Drury, C. Tan, M. and Helmers. 2019. Towards improving the DNDC model for simulating soil hydrology and tile drainage. 2019 ASABE Annual International Meet, Boston, Massachusetts, July 7–10. DOI:https://doi.org/10.13031/aim.20

Smith, W., B. Grant, W. He, Z. Qi, and A. VanderZaag. 2019. Modelling approach for identifying management practices that reduce GHG emissions from cropping systems in Canada. Proceedings of the workshop on "Climate change, reactive nitrogen, food security and sustainable agriculture", Garmisch-Partenkirchen, Germany, 15-16 April, 2019.

Smith, W., Z. Qi, and B. Grant. 2019. Improving Canada DNDC for simulating water quality and GHG emissions from cropping systems. Agricultural Greenhouse Gas Program meeting, McGill University, Macdonald Campus, Ste Anne de Bellevue, Quebec, January 16, 2019.

Smith, W., Z. Qi, B. Grant, A. VanderZaag, and R. Desjardins. 2017. Comparison of DNDC and RZWQM2 for simulating hydrology and nitrogen dynamics in a corn-soybean system with a winter cover crop. American Geophysical Union, Fall Meeting 2017. 2017AGUFM.B53B1959D

Smith, W., B. Grant, A. VanderZaag, Z. Qi, C. Drury, R. Desjardins, E. Pattey, B. Dutta, and G. Guest. 2016. Overview of Canada DNDC model development and studies pertaining to crop water use and nutrient loss. China-Canada Water Resource Workshop, Ottawa, ON, Canada, November 15th, 2016.

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Nomenclature

Commonly used abbreviations, acronyms and symbols are listed below. Other symbol definitions appear with equations in the text.

BMP	beneficial management practice
B	broadcast fertilizer
C	carbon
CO_2	carbon dioxide
CC	cover crop
CDS	controlled drainage with sub-irrigation
d	Wilmott index of agreement
DayCent	daily version of the Century model
DNDC	DeNitrification–DeComposition
DNDC.vCAN	Canadian version of the DNDC model
DSSAT	Decision Support System for Agrotechnology Transfer
ET	evapotranspiration
PET	potential evapotranspiration (reference ET adjusted using crop coefficient)
F	fall
GCM	global climate model
GDD	growing degree days
GHG	greenhouse gas
i	injected fertilizer
I	incorporated fertilizer
K	hydraulic conductivity
KSAT	saturated hydraulic conductivity
MS	maize-soybean rotation
M	mineral fertilizer (inorganic)
N	nitrogen
N_2O	Nitrous oxide
NH_3	ammonia
NH_4^+	ammonium

NO_3^-	nitrate
NARE	normalized average relative error
NRMSE	normalized root mean square error
NSE	Nash-Sutcliffe modelling efficiency
NCC	no cover crop
O	organic fertilizer
PET	potential evapotranspiration
r^2	Coefficient of determination
RMSE	root mean square error
RZWQM	Root Zone Water Quality Model
RCP	representative concentration pathway (IPCC climate scenario)
RCP4.5	4.5 Wm-2 radiative forcing climate change scenarios
RCP8.5	8.5 Wm-2 radiative forcing climate change scenarios
S	spring
Sd	side-dress fertilizer addition
SM	soybean-=maize rotation
SOC	soil organic carbon
Sp	split fertilizer addition
SWC (θ)	soil water content
TD	tile drainage (unrestricted)
WFPS	water filled pore space

Chapter 1

Introduction

1.1 Background

Effective agricultural management of cropping systems is required to enhance the profitability for producers and to reduce the environmental impact of pollutants, such as GHG emissions, which cause global warming (IPCC, 2018), nutrient losses which can cause eutrophication within water bodies (Chislock et al., 2013), and ammonia loss which can increase fine particulate matter in the atmosphere (Behera et al., 2013). In Canada, ammonia losses were estimated to be 306 kT N in 2011 (Sheppard and Bittman, 2016) whereas annual losses of N_2O from Canadian agriculture was estimated to be 74 kt N (Worth et al., 2016). Average annual N losses to groundwater in Canada are estimated to be ~161 kt N based on annual losses of 3.7 kg N ha^{-1} across the country (De Jong et al., 2009). Nutrient loss is reported to be very low for western Canada which constitutes about 80% of the agricultural land area but can range up to 45 kg ha^{-1} in some eastern provinces. Using base calculations from Sheppard and Bittman (2016) the total combined N losses from ammonia volatilization, N_2O emissions and drainage represents ~27% of the value of fertilizer shipped to farms or a cost of $707 million. A much larger cost could be expected in response to environmental damage and harm to human health.

From years of experimental research, Canadian scientists have helped to quantify the long-term sustainability of these agricultural systems by studying the interactions between climate-plant-soil, and management (Tenuta et al., 2019: Woodley et al., 2018). The challenge has been to how best incorporate this knowledge into a platform that can facilitate the investigation of integrated management solutions for a diverse agricultural landscape. Ideally, these solutions must be ones that promote the resiliency of agricultural systems while minimizing nutrient losses and improving soil health and productivity. Agroecosystems contain tightly coupled nutrient and energy flows, therefore assessment of these systems is challenging as they are composed of a complex array of dynamically linked processes that need to be considered concurrently in order to properly assess management impacts. Because process-based agricultural models dynamically simulate many of the interdependent process over space and time while maintaining the mass balance of nutrients and water, they are needed for predicting nutrient losses in the environment and assisting in the selection of BMPs (De Jong et al., 2009). However, these models do have recognized knowledge gaps and thus the analysis of new targeted measurements and the development of new algorithms for models are essential to ensure that the iterative process of model development continues. It is important that models consider the interactions within the soil-plant-atmospheric water cycle and the current state of knowledge regarding nutrient transformations, transport and losses.

A number of process-based (biophysical) agricultural models have been developed which consider crop growth and phenology, hydrological processes, nutrient transformations, cycling and transport. Each of these models has their advantages and disadvantages. Empirical or statistical models can also be useful but generally can't be employed beyond the range of information used in their development and parameterisation. Most models are developed to specialize in one outcome such as crop biomass, GHG emissions, soil carbon change, or water quality but all of these outcomes are linked and a model needs to consider them concurrently in order to assess trade-offs in climate and management impacts. In doing so there is risk of process interactions becoming very complex reducing transparency to the scientific and agricultural community and a risk of limiting the applicability of the model. Thus there is a balancing act required and developers often choose simplified processes to keep the user expertise, input requirements, transparency and computation time manageable. Some of the more frequently used models in North America include The Environmental Policy Integrated Climate Model (EPIC; Izaurralde et al., 2012), The Decision Support System for Agrotechnology Transfer (DSSAT; Hogenboom et al., 2017), DayCent (del Grosso et al., 2011) which is a daily version of the CENTURY soil carbon model expanded to simulate crop biomass and trace gas emissions, the Root Zone Water Quality Model (RZWQM2; Ma et al., 2012) and the DeNitrification DeComposition model (DNDC; Li et al., 1992, 2012).

The DNDC model is widely used, includes a very wide range of biogeochemical processes (Brilli et al., 2017; Gilespy et al., 2014; Giltrap et al., 2010) and is arguably the most sophisticated for estimating GHG emissions, however, the model demonstrates weaknesses in simulating soil hydrology and the overall water budget and does not include mechanistic tile drainage (He et al., 2018a; Brilli et al, 2017; Dutta et al., 2016b; Uzoma et al., 2015; Congreves et al., 2015b; Cui et al., 2014; Abdalla et al., 2011; Deng et al., 2011; Smith et al., 2008). Previous versions of DNDC employed a simplistic empirical relationship or "recession curve" to delay drainage by soil layer (Li et al., 2006), but this recession curve required parameterization of coefficients for each soil type, and is no longer active in the current release version. Li et al. (2006) also included a “deep water pool” to increase the default 50 cm soil profile depth to that of a tile drain; however, the deep water pool cannot be adjusted in depth and N transformations are not included. There are ongoing efforts to develop a Canadian version of the model (DNDCv.Can) which includes improved biogeochemical processes and growth characteristics for crop cultivars grown in Canada. However, the simple representation of water dynamics in the model still adversely impacts performance and the model cannot simulate drainage design impacts. Since the model is needed for performing agri-environmental assessments within Canada and its now being used by several research institutions globally it is crucial that it be updated for simulating soil hydrology. This will expand the model’s capabilities for assessing agricultural management impacts on cropping systems across a wider range of soils, climates and sustainability metrics. It is also important that modeller expertise be expanded and that plausible modeling approaches be developed to lower uncertainty in estimates. This is especially critical when considering potential impacts of agricultural practices on cropping systems under climate change which adds an additional level of complexity.

1.2 Objectives

The primary goal of this research was to improve a well-known biogeochemical model, DNDC, for simulating soil hydrology and tile drainage to enable a more robust and complete exploration of beneficial agricultural management practices that may mitigate adverse environmental impacts, both currently and under future climate change. Specific objectives corresponding to four journal articles are as follows;

i. To compare the performance of the default DNDC model, which utilizes simplified expressions for water dynamics to the more hydrologically complex RZWQM2 using a detailed dataset of crop biomass and N uptake, soil water content, drainage, and N loading to tiles. Recommend improvements to DNDC.

ii. To revise hydrologic processes in the DNDC model by including a new tile drainage sub-model, ability to simulate controlled drainage and sub-irrigation, improved soil water flow, a heterogeneous soil profile, revised root penetration and density functions, and a deeper soil profile. Compare the performance of the revised DNDC model to RZWQM2 using detailed datasets of runoff and drainage in eastern Canada and the US Midwest.

iii. To use the revised DNDC model to investigate inorganic and organic fertilizer management practices over a 30 year time horizon to determine practices which may reduce reactive N loss from corn silage production in cool climatic zones of eastern Canada and the US Midwest and to examine trade-offs and synergies between N loss to tile drains, N loss to runoff, NH_3 volatilization and N_2O emissions. Recommend beneficial management.

iv. To investigate the implications of using simpler versus more advanced modelling approaches for simulating the impacts of climate change on crop production, SOC change, N_2O emissions and N leaching and runoff and recommend an approach under cool weather climates. Assess the effect of climate change on crop production and sustainability for common cropping systems in Canada.

1.3 Thesis structure

The thesis is presented in a “manuscript based” style whereby the general introduction is provided in Chapter 1 which includes the research background and gaps in knowledge, the objectives and thesis outline. Chapter 2 provides a literature review of the development and application history, strengths and weaknesses and processes simulated in the DNDC model as well as a summary of hydrologic processes included in RZWQM2 and an overview of alternative soil hydrologic processes that could be employed to improve DNDC. Chapters 3, 4, 5, and 6 present the research in accordance with objective 1, 2, 3 and 4, respectively, with each chapter consisting of a research paper. Connecting text is provided to link the research. The papers are formatted according to the requirements of Library and Archives Canada. Supplementary tables and figures are provided at the end of each paper since they appear with the papers online and are referred to often. All references are located at the end of the thesis.

Chapter 2

Literature review

2.1 Overview of the DeNtrification DeComposition model (DNDC)

The DNDC (Li et al., 1992, 2012) model is a widely used process-based model developed originally to simulate N_2O emissions and quickly gained attention due to its detailed biogeochemical equations for describing nitrification and denitrification processes. The most recent release version is DNDC95 (http://www.dndc.sr.unh.edu/). It includes several sub-models for predicting crop growth, soil climate, decomposition, nitrification, denitrification, and fermentation. The model was first developed to estimate trace gas emissions (Li et al., 1992), but was later expanded to estimate soil C&N cycling (Li et al., 1994), water drainage and nitrogen movement (Li et al., 2006), phenological-based crop growth (Li, 2000) and finally to include full farm facility and livestock systems (Li et al., 2012). The model has been tested and validated extensively for simulating crop growth, GHG emissions, soil carbon change, and ammonia volatilization worldwide (Ehrhardt et al., 2018; Brilli et al., 2017; Zhang and Niu, 2016; Gilhespy et al., 2014) but it has seldom been tested for simulating water flow and nutrient losses to tile drains. Giltrap et al. (2010) provides a general overview of DNDC mainly in relation to simulating GHG emissions, while Zhang and Niu (2016) document the progression of the crop sub-model development in DNDC and reviews applications for simulating C&N cycling and GHG emissions (Zhang and Niu, 2016). Further, a review of nine C&N models that simulate trace gas fluxes found that DNDC was the only model which estimated all C&N related GHG emissions considered (Brilli et al., 2017). The most common problem contributing to poor accuracy in these models was reported to be poorly defined pedo-climatic conditions. The models employed simplified soil hydrology and the soil profile was often not well characterized.

The DNDC model framework is composed of several major components characterizing the soil climate, crop growth and development, organic matter decomposition, denitrification, nitrification, and fermentation (Fig. 2.1). A core strength of the modelling framework is in its ability to characterize a wide array of crop management activities while enforcing a mass balance of nutrient and water budgets. The model is a full farm system model, being able to simulate not only plant processes, including competition from crops grown simultaneously, but also enteric fermentation and other digestive processes in livestock, and C&N&P cycling in barns, manure lagoons, composters, and digesters (Li et al., 2012; Guest et al., 2017b). In a survey of 98 users Gilhespy et al. (2014) found strengths to be its ease of use, the availability of default parameters for 60+ crop types, and a large number of outputs. Main weakness were that soil-crop-atmospheric processes were not well documented in the user's manual and the lack of availability of the source code. Gilhespy et al. (2014) also provides a history of the last 20 years of DNDC developments including an overview of the "family" of DNDC models for simulating cropping systems in various regions worldwide. The DNDC model was originally developed in the U.S, but several modelling teams later created specific versions to better enable the simulation of regional soils, climate events, crop cultivars and management practices in the UK (Brown et al., 2002), New Zealand (Giltrap et al., 2008), Germany (Haas et al., 2013), Europe in general (Leip et al., 2008), China (Jiang et al., 2018c) and Canada (Kröbel et al., 2011). There is recent effort in the U.S. to develop an open source version of DNDC whereby developments from the other model versions which simulate cropping system dynamics can be merged (Salas, W., 2019; personal communication). Also, DNDC has been coupled with several other models for simulating detailed physiological responses in crops (Crop-DNDC; Zhang et al., 2002) forest systems (Forest-DNDC; Li et al., 2005), wetland systems (Wetland-DNDC; Sun et al., 1998), and economic assessments of farm systems (EFEM-DNDC; Neufeldt et al., 2005).

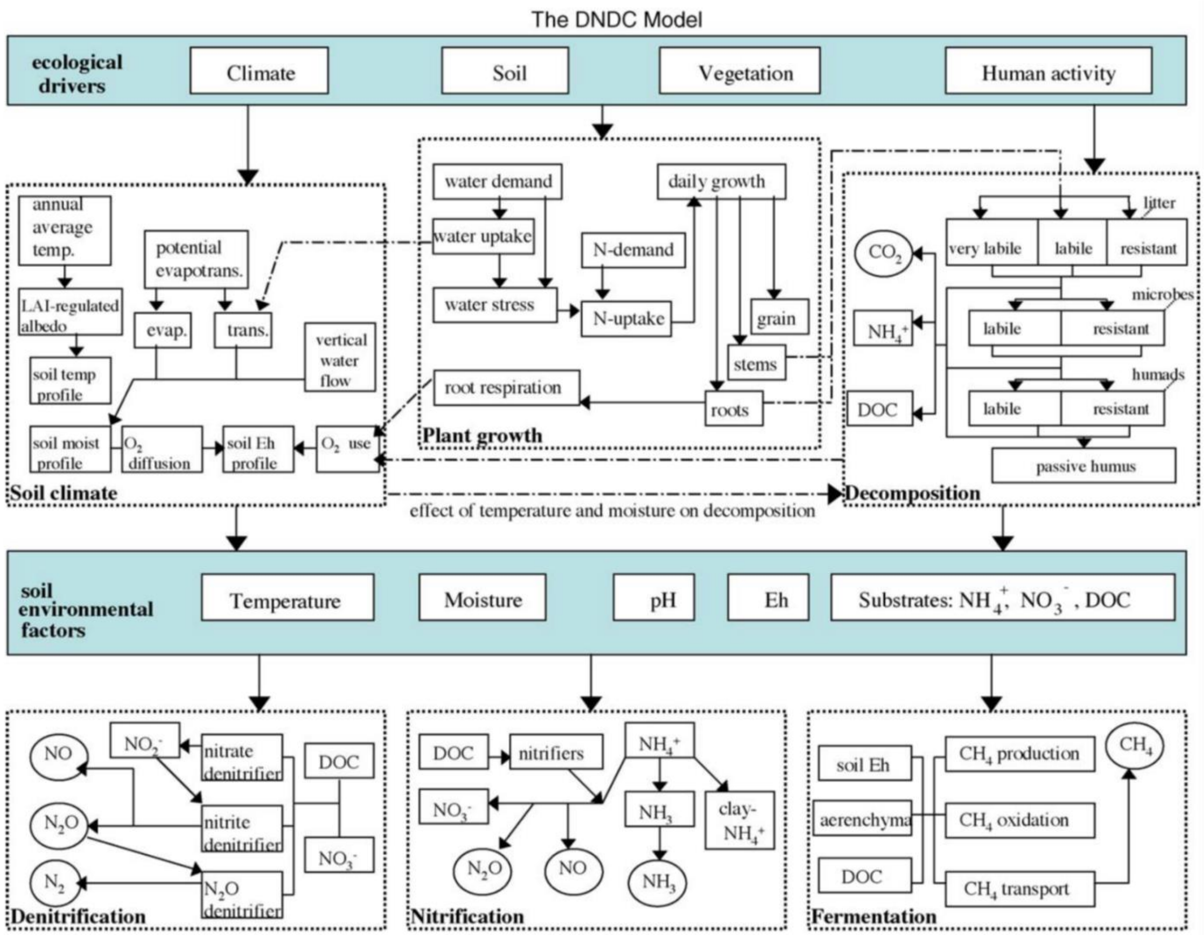

Figure 2.1 DNDC model structure showing main sub-models and processes bridging ecological and soil environmental drivers. The model features shown remain intact in the model today but have in some cases been expanded to include more robust description of processes and C&N&P cycling in livestock and farm facilities. Adapted from Li et al. (2006) and Gilhespy et al. (2014).

2.1.1 Canada DNDC (DNDCv.CAN); implications of past developments and future requirements

The Canadian version of the model (DNDCv.CAN) which is used as the starting point for development in this thesis has been under development since 2011, originally to improve the simulation of crop cultivars and agricultural management in cool weather climates (Kroebel et al., 2011) but more recently to expand the model's functionality for simulating additional management interactions and to integrate more robust mechanisms. The developments since 2011 along with several applications for simulating GHG mitigation, soil carbon change, and nutrient losses from cropping systems are documented in 25 peer reviewed journal articles (https://www.globaldndc.net/information/publications-i-3.html). Focus has recently been placed on improving the simulation of crop growth and development, soil physical processes and reactive N losses with little focus on hydrology. It is now necessary that the simulation of soil hydrology be improved before the more complex microbial and chemical processes affecting nitrification, denitrification and decomposition can be addressed (Uzoma et al., 2015; He et al., 2018a).

Table 2.1 Canada DNDC model developments that contribute towards improved estimates of C&N cycling and trace gas emissions.

Soil Physical Processes	**Biochemical Processes**	**Crop Processes**
Soil Temperature (snow cover, biomass, residue, soil texture)	Improved NH_3 Volatilization for manure slurry and urea	Evapotranspiration (K_{Crop} ET calculations, crop specific growth curves)
Dynamic soil physical characteristics	Included soil pH buffering	Root Dynamics (Root Density & Depth Functions)
Improved deep profile storage of water and N	Added Fert-N Inhibitor dynamics	Improved Nitrogen Fixation (Apsim adaptation)
	Soil C&N cycling (manure decomposition *f* of C:N ratios)	Added Winterkill and Perennial Growth functions
		Improved CO_2 effects, revised temperature crop stress

Several developments are summarized in Table 2.1 which were implemented into Canada DNDC and had notable impacts on soil C&N cycling and trace gas emissions. These included i) crop growth was improved by including crop-specific growth curves to regulate N and water demand for cool weather cultivars including regrowth of perennials and winterkill impacts

(Kroebel et al., 2011; Grant et al., 2016; He et al., 2019a), ii) temperature stress on crops was reformulated to be based on cardinal temperatures, the effect of exposure to high temperature during anthesis on harvest index and the effects of CO_2 fertilization on C assimilation, water and N use efficiency were included (Smith et al., 2013), iii) transpiration algorithms were reformulated to be based on daily water demand requirements of crop production and a crop coefficient approach was adopted to adjust the reference evapotranspiration estimated through the Penman–Montieth equation to potential evapotranspiration (PET) as denoted in DNDC (Dutta et al., 2016b), iv) a new sub-model was developed for predicting NH_3 volatilization from slurry (Congreves et al., 2016b) and urea accompanied by soil pH buffering (Dutta et al., 2016a), v) the ability of the model to characterize effects of management practices, snow cover, and soil texture on soil temperature was improved (Dutta et al., 2018). In undergoing these developments some of the more sensitive N_2O, NH_3, an soil N related parameters (i.e. growth and death rate of nitrifiers and denitrifiers, nitrification rate, and spring thaw microbial activity) are now located in the model input interface to allow for adjustment during calibration phases. Previously in DNDC95 these could only be modified within the code which resulted in different versions of DNDC with markedly different results. All developments for Canada DNDC noted in Table 2.1 were incorporated into the U.S. release version thus creating an up to date model version which included both the U.S. and Canadian developments (Smith et al., 2019c). This is the model version we further develop in this thesis to include improved soil hydrology and tile drainage.

2.1.2 Soil hydrologic processes in DNDC

At the time of the initiation of this thesis DNDCv.CAN used virtually the same below ground water processes as DNDC95. Efforts are made by the model developers to minimize the amount of input data and process time required thus some of the processes in DNDC were purposefully kept simple. DNDC employs a cascade flow water model simulating bulk water flux and N transport through the profile (Table 2.2; Fig. 2.2). In the sub-model for thermal-hydraulic flow, all soil water dynamics are calculated on an hourly time step using a layered water budget approach. The soil profile is divided into horizontal layers with thicknesses ranging from 1.5-3 cm, with lower layer thickness at higher clay content. Precipitation and irrigation are added at midnight at constant intensity, and therefore of variable duration (Li et al., 1992). Canopy interception and runoff (SCS curve number approach) are also calculated on an hourly basis. Infiltration occurs at a max rate of K_S, layer by layer, with field capacity being the upper limit of water holding capacity. Precipitation is assumed to be snow when air temperatures drop below 0°C and it accumulates on the soil surface. Ponding of water can occur if soil is frozen or if the rate of infiltration exceeds K_S. This water is susceptible to runoff. Evapotranspiration is calculated using a Penman–Montieth approach with a coefficient for each specific crop type to adjust reference evapotranspiration to PET (Dutta et al., 2016b). The water demand of the crop is based on the "crop water use" parameter, the growth curve, and the crop coefficient (Dutta et al., 2016b). Transpiration is based on the crop water demand but is limited by soil water status. Transpiration is determined first, with a minimum of 10% potential evapotranspiration reserved for evaporation. Evaporation from the soil, leaves, and stem are then calculated as a function of the remaining PET.

Table 2.2 Hydrological processes used in DNDC95 and DNDCv.CAN

Hydrology component	Process description
Soil profile	Homogeneous soil properties to 50 cm depth, layers ~2 cm thickness, underlying deep water pool form 50 to 100 cm depth.
Soil water transport	Water drains between soil layers if above field capacity (cascade "tipping bucket" flow)
Infiltration and runoff	Runoff is removed based on the SCS curve number method, followed by Canopy interception, then infiltration is limited by surface saturated hydraulic conductivity (K_{SAT}).
Potential Evapotranspiration	Penman-Monteith FAO approach where reference evapotranspiration is adjusted with coefficients for each crop type, Transpiration is a function of PET and crop water uptake demand determined by biomass
Tile drainage	Bulk gravity drainage with no deep seepage considered
Water table	None simulated

Li et al. (2006) included a "deep water pool" in DNDC to increase the default 50 cm soil profile depth to that of a tile drain; however, the deep water pool cannot be adjusted in depth without recoding the model and N adsorption and transformations are not included in this additional profile. Grant et al. (2016) expanded the functionality of the deep water pool by allowing for the water holding capacity to be adjusted based on bulk density. Adsorption and desorption of NH_4^+ based on the Langmuir equation was also incorporated in his study as well as a simplistic empirical relationship or "recession curve" to delay drainage by soil layer. This recession curve required parameterization of coefficients for each soil type (Toniito et al., 2007a), and is no longer active in the current release version (Smith et al., 2019c). Tonitto et al. (2007a,b) found that after calibration of the recession equation in DNDC the model performance was satisfactory for simulating annual water flow and nitrate loss to tile drains when aggregated across a watershed; however, DNDC consistently under-predicted peak monthly drainage events and the model was not tested using daily data.

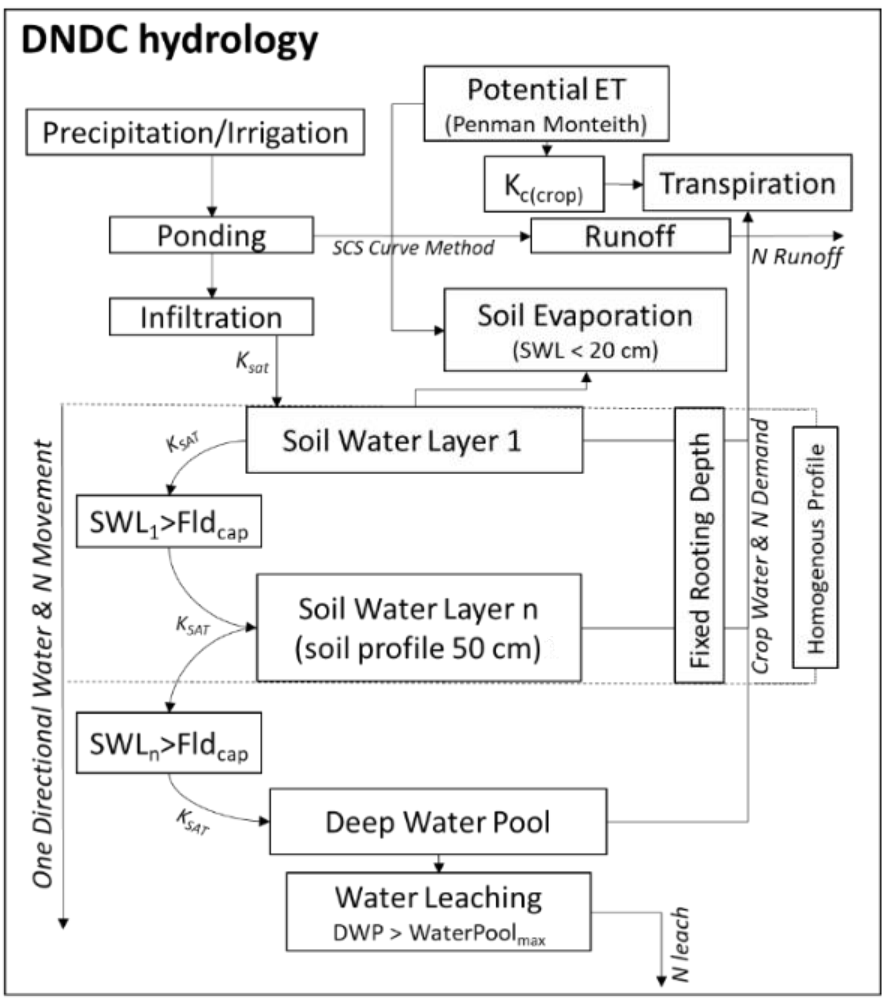

Figure 2.2 Schematic of hydrological processes in DNDC and DNDCv.CAN

In a study by David et al. (2009) 6 models (SWAT, DayCent, EPIC, Drainmod-N II and two versions of DNDC, 82a and 82h) were compared for simulating aggregated water and nitrate flux to tile drains. It was found that all models except DNDC82h performed well in simulating monthly water flux, but the models which were designed to simulate tile drainage (SWAT, EPIC and Drainmod-N) demonstrated better performance. All of the models investigated included a cascade flow approach to simulating drainage. At this time the DNDC model versions tested included a Thornthwaite method for estimating evapotranspiration which could sometimes overestimate losses, thus it is not surprising that DNDC underestimated water loss to drains. The current DNDC95 and DNDCv.CAN models includes the Penman-Monteith approach for evapotranspiration with crop specific coefficients, added in a joint US-Canada effort (Dutta et al., 2016b). It is very important to simulate an appropriate level of ET, since it is often the largest component of water loss, especially in semi-arid climates. Recent studies in Canada have shown that DNDCv.CAN performed better than some water budget models (Guest et al., 2018) for simulating soil water content, evapotranspiration and water loss to tiles and performed similarly to other cascade models (Guest et al., 2017a) for simulating soil water content, but all models demonstrated flaws.

2.1.3 Nitrogen processes in DNDC

2.1.3.1 Nitrogen leaching and runoff

Nitrogen in DNDC can be supplied through fertilizers, mineralization, deposition, and biological N_2 fixation. The original nitrate movement in DNDC was conceived as a function of the water flux per layer (Li et al., 2006). Soil NO_3^- was considered to be mobilized by positive water flux (90% mobilized) and transferred to the layer below as a one-dimensional vertical N flux towards the bottom soil profile. The movement of NO_3^- is an iterative step through each of the saturated layers per hour. Ammonium adsorption to clay (based on the Langmuir adsorption isotherm) also restricts N mobility since there is less nitrification with less NO_3^- available in solution. Additionally, another fraction (10% of the NO_3^- in each layer) was considered to be lost through preferential water flow via macropores directly out of the soil profile. Nitrate fertilizers are added directly to the soil NO_3^- pool thus they may be more subject to more initial leaching. Urea is moderately mobile in the model whereas NH_4^+ is not mobile. Ammonium-based fertilizers undergo nitrification to NO_3^- before movement can occur and urea undergoes hydrolysis to NH_4^+ followed by nitrification to NO_3^- (Dutta et al., 2016a). In the default U.S. release version of DNDC NO_3^- travels through the profile in solution, and is leached from the 50 cm depth.

To estimate runoff DNDC uses the SCS runoff curve number method developed by the USDA Natural Resources Conservation Service (Table 2.2). Nitrogen loss to runoff in DNDC is calculated as a fraction of rainfall that goes to runoff (based on SCS method) multiplied by the nitrate found in the top surface layer (~0.5 - 2 cm), simulated on a daily time step (based on inspection of DNDC code). An option could be to incorporate the Green-Ampt infiltration equation (Green and Ampt, 1911) which may improve the estimation of water and N runoff. The accurate simulation of runoff is, however, complex particularly when surface crusting, clay cracking, preferential flow through insect and root channels, snow dynamics, and soil freeze-thaw are prevalent.

The DNDC95 model has been employed to estimate drainage and N loading to tiles in the US (Li et al., 2006; Tonitto et al., 2007a, 2007b, 2010; Gopalakrishnan et al., 2012) and China (Li et al., 2014; Zhao et al., 2014) and once calibrated the model generally performed well, however, the model was not tested systematically for simulating crop biomass, soil water content, and daily water flow in these studies. Neither DNDC95 or DNDCv.CAN have been tested for simulating N loading to tiles in Canada.

2.1.3.2 Nitrous oxide emissions

In DNDC nitrification and denitrification processes are characterized in the "anaerobic balloon" sub-model (Li et al., 2012). The algorithms in DNDC.vCAN remain identical to those in DNDC95. The "anaerobic balloon" concept uses the Nernst equation to estimate redox potential (Eh) which regulates the size of the anaerobic (denitrifier) and aerobic (nitrifier) microbial fractions. The anaerobic portion is considered to be inside the balloon and the aerobic outside. The nitrification rate is determined as a function of nitrifier bacteria biomass, NH_4^+ concentration, a temperature reduction factor, a moisture reduction factor and pH. The N_2O from nitrification is regulated by water filled pore space, quantity of N nitrified, and temperature. In addition to determining when nitrification and denitrification occurs the Nersnt equation determines when specific biologically mediated reductive identification reactions occur, from $NO_3 \rightarrow NO_2 \rightarrow NO \rightarrow N_2O \rightarrow N_2$. The rate of the reactions (microbial growth) is then determined using the Michaelis–Menten equation, a multi-nutrient dependent growth function dependent on temperature, dissolved organic carbon, soil water, Eh, and pH. N_2O from denitrification is calculated as stepwise transformation process as a function of microbial growth and pH.

The redox potential is estimated as follows:

$$E_h = E_o + \frac{RT}{nF} * \ln\left(\frac{[OX]}{[RE]}\right) \tag{2.1}$$

where E_h is the redox potential (volts), E_o is the standard half-cell reduction potential (volts), R is the is the universal gas constant, T is the temperature in kelvins, F is the Faraday constant, n is the number of electrons transferred in the redox reaction, and OX and RE are concentration of oxidant and concentration of reductant (mol/L), respectively.

In the denitrificiation submodel, the quantity of denitrifier-bacteria is estimated using a multi-nutrient dependent (Michaelis–Menten) growth function dependent, kinetically determining the growth rate as follows:

$$R = R_{max} * \frac{DOC}{K_a + DOC} * \frac{OX}{K_b + OX} \tag{2.2}$$

where R is the growth rate, R_{max} is the maximum growth rate, DOC is concentration of dissolved organic carbon, and K_a and K_b are half-saturation for substrates DOC and OX, respectively. The constants and Rmax were taken from a laboratory study by Leffelaar and Wessel (1998). More information on the growth and death rate of nitrifiers and denitrifiers can be found in Li et al. (2012).

DNDC was primarily developed to estimate N_2O emissions and the model is currently used worldwide for this purpose. It has recently performed well for simulating seasonal emissions. For instance in a blind global study to estimate crop yields and N_2O emissions using 24 models, DNDC performed within the top three models for each of the three annual crops simulated (Ehrhardt et al., 2018). However, in this study comparisons were made using only cumulative seasonal emissions and the timing of emission events were generally not well simulated. This was also the case for several recently published studies using DNDCvCAN, whereby the seasonal sum of N_2O emissions was generally well simulated in comparison to measurements (He et al., 2018a, 2019b; Grant et al., 2016; Uzoma et al., 2015; Smith et al., 2008), however, the timing of daily emissions was more difficult to replicate. It should be noted that the experimental variability when measuring N_2O emissions using chambers can sometimes be high and gap filling is required to estimate daily emission levels based on a 30-45 minute sample. However, there remain several limitations in the modeling framework that need to be resolved to reduce uncertainties. For instance, it was found that DNDC underestimated N_2O emissions during long periods of episodic rainfall due to the inability of a cascade flow model to simulate water content above field capacity (Uzoma et al., 2015) which strongly influences oxygen diffusion into the soil and the type of denitrification reactions that occurs (Butterbach-bahl et al., 2013).

To partially compensate for this deficiency, the reactions from nitrate to N_2 in DNDC are currently set to occur in the range from wilting point to field capacity, but Butterbach-Bahl et al. (2013) indicate that N_2O production should occur above field capacity, usually at about 80% WFPS. Improvement of the water model will allow for adjustment of the reduction reaction to occur at the proper redox potential (N_2O typically occurs above field capacity). This will in turn allow for removal of a rainfall multiplier in DNDC which was assumedly applied to increase N_2O emissions during times of high soil water content.

Also, DNDC does not separately characterize N_2O production and consumption (Wen et al., 2016) processes and diffusion is only handled in a simplistic empirical manner. These processes are also impacted by soil water content and soil N availability. Thus a main weakness in the model for simulating N_2O emissions and other trace gases remains its simplistic and often inaccurate simulation of soil hydrology and the overall water budget (Brilli et al, 2017; He et al., 2018a; Dutta et al., 2016b; Uzoma et al., 2015; Congreves et al., 2016b; Cui et al., 2014; Abdalla et al., 2011; Deng et al., 2011; Smith et al., 2008).

2.1.3.3 NH_3 volatilization

The U.S. release version of DNDC originally included a NH_3 volatilization sub-model (Li et al., 2012) based on acid–base equilibrium principles (Petersen et al., 2014), however, this sub-model was improved in DNDCv.CAN whereby it operates on an hourly time step, includes more manure inputs, and includes revised expressions for NH_3 volatilization from the soil surface (Congreves et al., 2016b). This sub-model is based on chemical equilibria principles whereby the acid–base equilibrium between NH_4^+ and NH_3 is determined in aqueous solution with the reaction rates being determined by the pH of the mixed soil solution and the dissociation constants influenced by soil temperature (Petersen et al., 2014). NH_4^+ adsorption by clay in the model also restricts mobility and limits availability for the acid-base equilibrium. The aqueous-gas equilibrium is then calculated using Henry's law with NH_3 volatilization being limited by a soil depth function. The utility of this development was further improved by Dutta et al. (2016a) who improved the simulation of urea hydrolysis and included the impact of buffer capacity on soil pH. Urea hydrolysis is determined as a function of N-urea concentration, volumetric moisture content, and a kinetic rate constant for hydrolysis. The pH buffering was derived from Tripathi et al. (2000) and is primarily a function of the cation exchange capacity of the soil.

2.1.4 Biomass growth and partitioning

In DNDCv.CAN, biomass growth is simulated using either a generalized crop growth curve based solely on GDD (Growing Degree Days - non-crop specific) or the recently integrated crop-specific growth (Kroebel et al., 2011; Grant et al., 2016; He et al., 2019a) whereby the phenological stages of plant growth for a specific cultivar are characterized by empirical growth curves specifying N requirements for C biomass accumulation and are driven by the accumulation of GDD. The current DNDC95 release version only includes the growth model that is based solely on GDD. There is a version of DNDC which includes a detailed phenological-based crop growth model (Zhang et al., 2002). Zhang and Niu (2016) provide details on the history of the crop model development in DNDC. In both DNDC95 and DNDC.vCAN the model tracks crop development using a plant growth index (PGI) that represents the ratio of the current GDD accumulated per total GDD required to reach plant maturity. This index is similar in scale to the BBCH phenology charts (Meier, 2001). The growth curves determine the daily N demand required for optimal daily biomass C accumulation and are a function of the overall plant C:N.

The plant biomass is divided into four crop fractions; grain, leaf, stem and roots. The relative fractions for leaf, stem and roots are constant during the vegetative portion of crop growth (crop specific period). Flowering and grain filling occurs at a predetermined PGI (crop specific) and the grain fraction increases linearly until it reaches the maturity target fraction for grain. The effects of CO_2 fertilization on biomass accumulation, water use efficiency and N use efficiency are included for C3 and C4 crops (Smith et al., 2013). Root, leaf, stem and grain respiration as well as LAI are calculated using the estimated net primary productivity (NPP).

GPP is the summation of the estimated NPP and total plant respiration. Ecosystem respiration is a sum of total plant and soil respiration.

The biomass C growth curves in DNDC are scaled based on the specified maximum potential grain yield input by the user. NPP is calculated based on this demand but is regulated by water, nitrogen and temperature stresses. The actual daily N demand and actual C growth is regulated by the available N in the soil profile, available soil water and further reduced by temperature stress. General temperature stress for crops is based on an equation that uses cardinal temperatures (minimum, maximum and optimum temperature for growth of each crop (Yan and Hunt, 1999). The effect of exposure to high temperature during anthesis on harvest index is also included for both wheat and maize (Ferris et al., 1998; Carberry et al., 1989). Evapotranspiration is estimated using the Penman Monteith equation, modified to include the FAO crop coefficient for four general crops types (small grain cereals, forages, legumes and oilseeds) (Dutta et al., 2016b). Crop water requirement (mm water per kg biomass) is crop specific.

Crop water stress is determined by estimating the actual transpiration (limited by available water)/potential transpiration (crop specific). A simple linear root growth function which can only extend to 50 cm depth determines the available soil profile that the crop can access for nutrient and water uptake during the season. Thus when the maximum rooting depth of 50 cm is reached the water and nutrient demand is partitioned evenly across the soil profile. The soil profile is modelled comprehensively for C&N dynamics to 50 cm depth but because it is not simulated below 50 cm DNDC sometimes simulates low mineralization which can impose excessive crop N stress (Grant et al., 2016; Smith et al., 2008).

2.1.5 Modelling studies to investigate BMPs for reducing N losses from cropping systems

Process based agricultural models can dynamically simulate many of the interdependent soil-plant-atmospheric processes over space and time while maintaining the mass balance of nutrients and water. Thus they are well positioned for the assessment of beneficial management practices (BMPs) that promote resilient, efficient and sustainable cropping systems (Brill et al., 2017; Ma et al., 2007a; De Jong et al., 2009). It is; however, crucial for modellers to work closely with crop agronomists to incorporate new knowledge and in some cases additional processes

(Vereecken et al., 2015) in order to be able to estimate trade-offs in environmental outcomes and ecosystem services.

A well calibrated model can be employed to simulate the long-term impacts of climate variability and management on N losses from cropping systems (Abalos et al., 2016b; Congreves et al., 2016a; Qi et al., 2011b). Although many agricultural models were originally developed to simulate a single output such as crop growth, soil carbon change, water quality, or GHG emissions, there has been increased effort to enhance models to include a larger scope of agricultural processes (Ma et al., 2007a). In many agricultural models, especially those focusing on crop growth, soil C dynamics and GHG emissions, soil hydrology is often handled in a rudimentary manner and tile drainage is not explicitly simulated (i.e. DNDC, DayCent, EPIC, DSSAT). Also, only a few models can mechanistically simulate certain processes such as NH_3 volatilization (Vereecken et al., 2015). Three models are predominantly used in the cooler regions of North America as they all characterize overwinter snow dynamics and soil freeze-thaw events. The DNDC model was originally developed to estimate N_2O emissions, whereas DayCent (del Grosso et al., 2001, 2011) focused more on soil carbon and RZWQM2 on water quality and crop growth. However all three models have been expanded to simulate all four outcomes.

The DNDC model has recently been employed worldwide to assess the impacts of BMPs on N_2O emissions (Chen et al., 2019; Deng et al., 2018; He et al., 2018b; Sándor et al., 2018; Molina-Herrera et al., 2016; Congreves et al., 2016a; Abalos et al., 2016b; Uzoma et al., 2015), however, few studies examine the trade-offs between reactive N losses (i.e. N_2O emissions, NH_3 volatilization, N leaching, N runoff). Molina-Herrera et al. (2016) performed a study using Landscape-DNDC to assess mitigation opportunities of N_2O emissions and N leaching for various agricultural sites across Europe. Congreves et al. (2016a) used DNDC.vCAN to examine the impacts of climate variability on N_2O emissions, NH_3 volatilization and N leaching losses in a conventional and best management cropping system at a site in eastern Ontario. However, N losses to tile drains was not explicitly simulated, although tile drainage was present at the research site. It is important that DNDC be improved for simulating water and N loading to tile drains since this is a principal practice in many regions of the world. The ability to simulate controlled drainage and sub-irrigation is also needed to enable the assessment of new technologies. Such improvements could further expand the ability to assess trade-offs in N losses for cropping systems.

2.1.6 Modelling climate change impacts on cropping systems

In most regions of the world it is likely that climate change will strongly influence crop growth and development, soil health, greenhouse gas (GHG) emissions and nutrient losses. In northern latitudes such as in northeast China and the UK some studies have found positive impacts on crop yields (Supit et al., 2010; Chen et al., 2010). A strong influence of climate change is expected in Canada where temperatures are increasing at a rate faster than the global average (Qian et al., 2019; Bush and Lemmen, 2019) and the estimated frost free period for crop growth has increased by approximately 3 weeks since the early twentieth century (Qian et al., 2012). However, in warmer regions globally crop growth may suffer under warmer temperatures. For instance, it was estimated that wheat and maize yields may already be declining, especially in tropical regions, with an estimated global average reduction of 5.5 and 3.8%, respectively (Lobell et al., 2011).

Food production using sustainable practices to maintain or increase crop yields while limiting negative anthropogenic influences on the environment is an important global research activity. It is becoming critical that we find ways to mitigate GHG emissions to limit global warming (IPCC, 2018). An increase in atmospheric concentrations of N_2O is primarily attributed to agriculture due to higher fertilizer use (IPCC, 2013: Tian et al., 2016) to meet food needs for a growing world population. Nitrous oxide concentration in the atmosphere has risen from 270 ppb in 1750 (IPCC, 2013) to approximately 330 ppb in 2017 (WMO, 2018). Higher N_2O contributes towards both increased global warming potential and stratospheric ozone layer depletion (Chipperfield, 2009; Denman et al., 2004). Since 1990 the radiative forcing of all GHGs has increased by about 41% (WMO, 2018). It is also important to account for changes in other adverse impacts such as nutrient losses that can cause eutrophication within water bodies, ammonia loss which increases fine particulate matter in the atmosphere and changes in soil carbon which impact soil health. Nitrogen losses from currently established cropping systems are generally projected to increase under future warmer climates, including N_2O emissions (Abalos et al., 2016a; Smith et al., 2013; Tian et al., 2012), NO_3^- leaching and runoff (Wang et al., 2015) and NH_3 volatilization (Suddick et al., 2012). To reach the increasing demands for food and fibre there will likely be increased N inputs in the future (Snyder et al., 2014) through expansion of agricultural areas and increased intensity, potentially further increasing N losses.

Statistical models are useful for estimating changes in yields and sometimes nutrient losses under current climate and management, however, they are not well suited for estimating the feedbacks from soil C&N cycling nor the complex physiological climate impacts on crop growth and development (Basso et al., 2015). The physiological effects of climate on crop growth need to be considered including the impacts of CO_2 fertilization on photosynthesis, water and N use efficiency, temperature and water stress during critical growth phases such as anthesis, and in the case of cool climates frost damage and winterkill (Smith et al., 2013). In order to simulate the impacts of changing stresses on crop production and nutrient losses it is important to include system feedbacks from water, C and N cycling thus a model needs to include robust hydrological and biogeochemical processes and be capable of simulating a wide range of agricultural management. When cool weather cropping systems are considered the impacts of snow cover and soil freeze-thaw dynamics are crucial (Cui and Wang., 2019; Dutta et al., 2018) for determining losses of water and nutrient to runoff and drainage, mechanisms which several prominent crop models currently do not consider. This may be partially why it is common practice in most climate change studies to re-initialize the soil status (water, soil organic carbon, nutrients) in models each year prior to the growing season (Basso et al., 2015) to avoid the issue. However, the soil status can greatly change over time resulting in significant feedbacks on crop growth (Basso et al., 2015) and environmental outcomes. Higher rates of N leaching and runoff often occur in the non-growing season when there is no crop water and N uptake (Smith et al., 2019a; Gamble et al., 2018; Schwager et al., 2015, 2016). Likewise, N_2O emissions are highly influenced by soil water status and can be strongly driven by off-season soil freeze-thaw activity in cool weather systems (Wagner-Riddle et al., 2008). Certain agroecosystem models such as DayCent, RZWQM2 and DNDC are capable of dynamically simulating many interdependent soil-plant processes under current and future climate and include over-winter soil freeze-thaw and snow dynamics.

Numerous Global Climate Models (GCMs) have been developed for simulating the circulation of earth's atmosphere. Many of these models have been used to project future climate in the Coupled Model Intercomparison Project Phase 5 (CMIP5; Taylor et al., 2012) and this data is available for download but a bias correction and downscaling procedure needs to be employed (Kirchmeier-Young et al., 2017; Cannon 2018) to enable its use in specific locations to drive agricultural models. The CMIP5 project projected climate change under several emissions scenarios consistent with the Representative Concentration Pathways (RCPs) released by IPPC (2014). The 4.5 and 8.5 Wm^{-2} RCP radiative forcing scenarios are commonly used in crop model assessment whereby the 8.5 Wm^{-2} scenario represents a future with relatively high GHG emissions (Van Vuuren et al., 2011; IPCC, 2014) and the 4.5 Wm^{-2} scenario which assumes some mitigation and social measures were employed to reduce GHG emissions.

Several modelling studies have been performed to assess the impacts of climate change on crop growth in Canada (Qian et al., 2019; Jarecki et al., 2018; He et al., 2018a,b; Smith et al., 2013) but few have attempted to understand changes in N losses such as N_2O emissions (He et al., 2018a; Smith et al., 2013), NO_3^- leaching, or NH_3 volatilization. This is partly because it is difficult to understand and develop robust soil C&N and hydrological processes required for tracking feedbacks between the plants, soil and the atmosphere, but also because there are inherent difficulties in understanding possible changes in agronomic practices which may occur and how to simulate them. For instance, in climate change studies it is crucial to modify fertilizer application rates over time in response to changes in crop N uptake requirements thus an algorithm needs to be developed which can be applied automatically in models.

2.2 Overview of hydrological processes in the Root Zone Water Quality Model (RZWQM2)

The RZWQM2 (version 3.0.2015; Ma et al., 2012) is a computational-based hydrology model which uses numerical solutions for determining water redistribution in the soil profile. RZWQM2 was developed to simulate detailed biogeochemical processes in cropping systems with a major focus on simulating water quality in the plant root zone, below the root zone, and also in runoff and tile drains. The model simulates a wide array of agricultural management and has recently been expanded and improved for simulating N_2O emissions (Fang et al., 2015; Jiang et al., 2019) and phosphorous dynamics (Sadhukhan et al., 2019). RZWQM2 includes DSSAT 4.0 crop models with CERES and CROPGRO components (Hoogenboom et al., 2017; Ma et al., 2005, 2006) which is a very well established framework for simulating crop growth and development worldwide. RZWQM2 uses a numerical solution to determine water fluxes and includes the Green-Ampt equation for infiltration, the Richards equation with an option for lateral hydraulic gradient for lateral water loss, and the Hooghoudt's equation for simulating quasi-2D tile drainage (Table 2.3; Fig 2.3). Thus the model input requirements, modeller expertise and computation time are greater than for DNDC. The model has been validated for simulating drainage and N loading to tiles at many locations in North America (Malone et al., 2017; Xian et al., 2017; Qi et al., 2011b; Li et al., 2008; Thorp et al., 2007; Akhand et al., 2003) and has been employed to investigate BMPs for reducing N losses.

Since RZWQM2 is a well-recognized model for simulating soil hydrology it offers an excellent opportunity for benchmarking DNDC developments. It has been employed previously to benchmark the performance of the HERMES model, which like DNDC uses a cascade water flow approach (Malone et al., 2017). It was found that HERMES did not simulate the year to year variability in nitrate concentration nor the monthly drainage as well as did RZWQM2. Refer to Jiang et al. (2018a,b) for detailed descriptions of processes simulated in RZWQM2, modes of operation and suggested parameterization, calibration and validation techniques.

Table 2.3 Description of hydrologic processes in RZWQM2

Hydrology component	Description
Soil profile	Heterogeneous soil properties, customizable soil profile to several meters depth
Soil water transport	Water redistribution simulated by Richards Equation, Brooks Corey soil-water characteristics curve, macropore flow option
Infiltration and runoff	Modified Green-Ampt approach to estimate infiltration rate, water excess goes first to macropores and then to runoff.
Potential Evapotranspiration	Modified Shuttleworth-Wallace model, constrained by water availability, multiple crop water stress options, reduces evaporation under residue-covered soil
Tile drainage	Hooghoudt’s equation, adjustable tile drainage depth, tile diameter, and drain spacing
Water table	Fluctuating water table

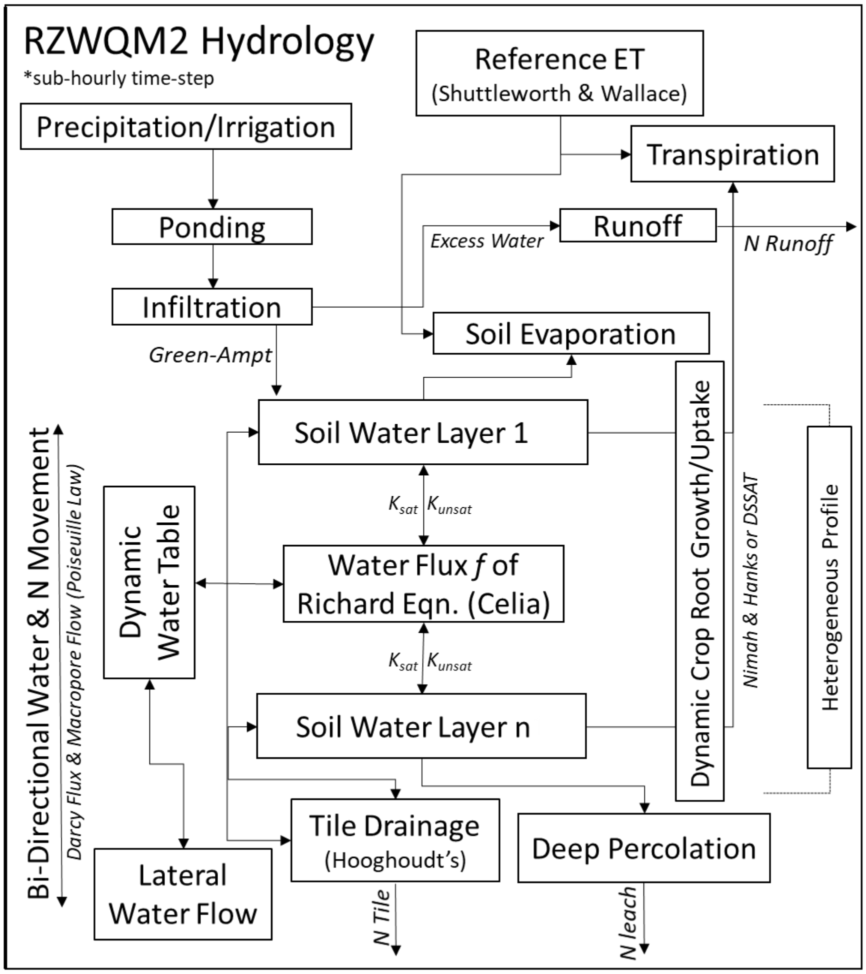

Figure 2.3 Schematic of hydrological processes in RZWQM2

2.3 Investigation of alternative soil hydrologic processes for improving the performance of DNDC

In this section focus is placed on researching alternative soil hydrologic processes for improving the simulation of subsurface soil hydrology in DNDC, the main weaknesses being the simulation of water movement and storage, water uptake by roots and tile drainage. In past studies focus was placed on improving the simulation of evapotranspiration (Dutta et al., 2016b), and snow accumulation and snow melt (Dutta et al., 2018).

2.3.1 Water redistribution in unsaturated soils

2.3.1.1 The Richards equation

Coupled hydrological models which include overland flow, unsaturated porous media, and groundwater flow have been researched for more than 50 years. In 1969 a blueprint was published providing an overview of numerical solutions and a guide for model development (Freeze and Harlan, 1969). Since this time increases in numerical and computational capabilities have enabled the development of integrated hydrological models for simulating surface and subsurface flow within catchments, sometimes developed in 1-D, 2-D or 3-D (Maxwell et al., 2015). Most of these models now include a solution which uses the Richards equation (Richard, 1931) which is a differential equation describing water movement in unsaturated porous media. Much research has gone into developing partial analytical solutions to Richards equation or into solving the equation using finite element and finite difference methods (Farthing and Ogden, 2017; Beven and Germann, 2013; Barari et al., 2009). The Richards equation is used in the majority of unsaturated flow studies and the equation can be expressed in 3 basic forms, based on soil water content (θ-based), pressure head (h-based) or mixed form (Hillel et al., 1980).

Head-based:

$$C(h)\frac{\partial h}{\partial t} = \nabla \bullet (K(h)\nabla h) + \frac{\partial K}{\partial z} \tag{2.3}$$

where C(h)[1/L] = $\frac{\partial \theta}{\partial h}$ is a function which describes the rate of change in moisture content in relation to the pressure head. Several curve fitting methods have been developed to describe the water content to pressure head relationships including van Genuchten (1980) which is described below. K[L/T] is the unsaturated hydraulic conductivity.

Saturation-based:

$$\frac{\partial \theta}{\partial t} = \nabla \bullet D(\theta)\nabla\theta + \frac{\partial K}{\partial z} \tag{2.4}$$

where D(θ)[L^2/T] = $\frac{K(\theta)}{C(\theta)}$ = K(θ) $\frac{\partial h}{\partial \theta}$ is the soil unsaturated diffusivity.

Mixed form:

$$\frac{\partial\theta}{\partial t} = \nabla \bullet K(h)\nabla h + \frac{\partial K}{\partial z} \tag{2.5}$$

2.3.1.2 Limitations of the Richards Equation for agricultural soils

Complex numerical schemes, such as finite difference and finite element solutions of Richards equation, can generally produce reasonably accurate results; however, such approaches can be computationally expensive (Farthing and Ogden, 2017; Short et al., 1995), partly because fine spatial discretization is required to simulate infiltration into dry soils (Downer and Ogden, 2004) but also because a small time step is required to simulate soils at high water contents and flow rates (Yang et al., 2009).

Intensive and accurate input data is also needed for fitting variables to represent a viable water retention curve (soil moisture characteristic) via the van Genuchten model or other curve fitting equation. The pressure plate method is commonly used for estimating water contents at a set pressure to determine the water retention curve. It can take weeks for the system to stabilize under high pressures but the results are generally accurate. However, at low water potentials this method is often inaccurate due to soil dispersion and lack of soil-plate contact (Bittelli and Flury, 2009) and the method can lead to substantial errors in flow calculations in models. There are other options such as the dew point measurement method whereby Kirstea et al. (2019) recently developed a method shown to provide accurate soil water retention data over the entire moisture range. Another issue is that it can be very difficult to get a good measure of *in situ* saturated conductivity particularly at deeper soil depths. Laboratory measurements of K_S using soil cores and the traditional saturated flow-desorption method can in fact be over an order of magnitude greater than *in situ* measured K_S (Smith et al., 1995). It is possible to use pedotransfer functions to estimate water retention curves and other hydrological parameters but in doing so it can undermine much of the improved accuracy that is achieved through using a computational-based water redistribution approach.

Further, there is some uncertainty regarding the applicably of Richards equation for agricultural soils. In a review of water flow approaches, Beven and Germann (2013) commented that in unsaturated heterogeneous soils there is rarely a consistent hydraulic gradient, which Richards equation assumes. In heterogeneous soils capillary potentials are not in equilibrium. In another review of numerical solutions for Richards' equation it was concluded that in certain conditions numerical solutions are still unreliable and that no robust approach exists across soils and boundary conditions (Farthing and Ogden, 2017). There are issues with convergence in more complex systems and they suggest additional research into alternative procedures.

2.3.1.3 Approximating Richards flow with simpler algorithms

To reduce the computation time needed to solve complex numerical schemes over spatial and temporal domains several researchers have worked on simplifying the Richards approach, but with attempts to maintain accuracy. A large number of researchers have developed analytical solutions but these can only be employed for simplified cases (Farthing and Ogden, 2017) thus are not functional for a wide range of transient conditions that occur in heterogeneous agricultural soils. For instance the quasi analytical method developed by Philip (1957) was one of the first approaches but it assumes a homogeneous soil and is employed to simulate ponded infiltration at the upper boundary. This method has since been integrated into other approaches such as recent differential equations developed by Ogden et al. (2015) which can simulate water flow through a heterogeneous profile. This approach conserves mass and has no convergence limitations but one drawback was that the computational requirement was similar to the Richards equation as employed in the Hydrus-1D model.

When developing the DayCent model Del Grosso et al. (2001) used a simple finite difference approximation whereby unsaturated water flow was estimated between layers discretized down the soil profile using the Darcy's equation with a damping flux rate to slow water flow. The damping flux rate, which could be determined based on calibrations using observed data, is set high to allow for larger time steps thus facilitating faster model performance. Matric potential is estimated for each time step using the Campbell method and water flux is simulated downward or upward. Water flow above field capacity is determined using a tipping bucket approach thus only unsaturated flow is estimated using the Darcy-damping flux approach. This approach is relatively simple and DayCent performed satisfactorily and marginally better than the DNDC and STICS models for simulating soil water at three sites in Eastern Canada (Guest et al., 2017a), however, the model was not tested against a comprehensive hydrology model.

Lee and Abriola (1999) used a derivation of the water-content-based Richards flow equation whereby it was assumed water content and pressure head were influenced only by the layer above and the layer below with discretization down the soil profile at a sufficiently low time step. This produced acceptable results for a homogeneous soil, however, was not applicable for flow between layers with varying soil properties (Yang et al., 2009). Yang et al. (2009) expanded on this approach using a mixed form of the Richards equation expressed in terms of soil water content and pressure head in a 1-D form as follows:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[K(\theta)(\frac{\partial h}{\partial z} + 1) \tag{2.6}$$

Integrating this form of the equation vertically over a soil layer Yang et al. (2009) derived the following;

$$\frac{\Delta \overline{\theta_i}}{\Delta t} = \frac{1}{\Delta z}\left[K_{i+1}\left(\frac{\Delta h_{i+1,i}}{\Delta z} + 1\right) - K_i\left(\frac{\Delta h_{i,i-1}}{\Delta z} + 1\right)\right] \tag{2.7}$$

where $\Delta\bar{\theta}_i$ (L^3L^{-3}) = the average soil water content in the layer i for the time step Δt and soil layer thickness Δz, K (LT^{-1}) is the hydraulic conductivity of the layer (i) and the above layer (i+1), and Δh (L) is the change in pressure head between the layers, i+1 being the layer above and i-1 the layer below. To estimate soil water retention characteristics for the integrated Richards equation Yang et al. (2009) employed the van Genuchten model (van Genuchten, 1980) but several other options which are explored below can be employed in hydrology models.

2.3.1.4 Estimates of soil water retention

The van Genuchten function is one of the more comprehensive soil water retention functions for estimating soil water content with respect to pressure head. The method is particularly useful for defining the shape of the curve near saturation and can be expressed relative to water content, pressure head (h; L), and unsaturated hydraulic conductivity (K; LT^{-1}):

$$\Theta = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \left[\frac{1}{1 + |\alpha h|^n}\right]^m \tag{2.8}$$

$$h(\theta) = \frac{1}{\alpha}\left(\Theta^{-1/m} - 1\right)^{1/n} \tag{2.9}$$

$$K(\theta) = K_s \Theta^{0.5}\left[1 - (1 - \Theta^{1/m})^m\right]^2 \tag{2.10}$$

where **Θ** is the relative saturation, θ_r and θs (L^3L^{-3}) are the residual and saturated soil water contents, α (L^{-1}) is a shape parameter related to the inverse of the air entry suction, n is a shape parameter related to the pore size distribution, m=1-1/n, and K_s (LT^{-1}) is the saturated hydraulic conductivity.

Several other options are available for estimating soil water retention curves including those proposed by Brooks and Corey (1964) and Campbell (1974) and more recently by Karup et al. (2017). The simplest model among these in its original form is the Campbell function (Pittaki-Chrysodonta et al., 2018) which only requires a pore size distribution curve-shape parameter (b) and the water content at the air entry value (bubbling pressure). The base principle for this function has been widely used in process-based hydrology models such as in the SHAW model (Flerchinger et al., 2000) but it has in some cases been expanded to include more detail. Hutson and Cass (1987) modified the equation to include two shape fitting parameters, one for a parabolic function at the wet end and a power function for drier conditions. This allowed for a better representation of soil water retention at near saturation and this was employed in the LEACHM model (Wagenet and Hutson, 1989). RZWQM2 uses a modified form of Brooks and Corey (Ma et al., 2012) to describe water retention and unsaturated hydraulic conductivity-matric suction relationships.

2.3.1.5 Cascade flow or tipping bucket approaches for estimating water movement

Many agricultural models such as DNDC, DayCent, STICS (Brisson et al., 2002), DSSAT (Hoogenboom et al., 2015), APSIM (Keating et al., 2003) and DRAINMOD (Skagg et al., 2012) employ a simple cascade water flow approach whereby water per layer "tips" to field capacity on a daily or hourly basis. It is recognized that this can result in erroneous predictions of soil water contents and flow events, however, the simple approach is often purposefully implemented to keep the computation time, soil data input requirements and level of required expertise low (Guest et al., 2018). However, without accurate soils data, especially to define the water retention curve, there is no guarantee that soil water content can be more accurately simulated using a more complex approach (such as by solving Richards equation numerically).

With a cascade approach there are clear issues in being able to simulate water contents that occur above field capacity which are typical during spring snow melt or long periods of episodic rainfall under cool climate (Uzoma et al., 2015). An option could be to limit water movement above field capacity based on some of the simpler equations which describe the unsaturated conductivity to pressure head relationship such those proposed by Brook and Corey (1964) or Campbell et al. (1974). Vereecken et al. (1990) tested these two models along with the three parameter Gardiner model (Gardiner et al., 1958) using 182 measured K(h) relationships and found the Gardiner model to be the best performer. They established regression equations whereby the parameters for Gardiner's model could be estimated based on simple soil properties such as K_S, soil texture, bulk density and carbon content. If the soil water status is known then unsaturated conductivity can be estimated based on soil water status and K_S as derived by both Averkjanov (1950) and Irmay (1954).

$$K = K_S\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^n \tag{2.11}$$

where K is hydraulic conductivity, K_S is saturated hydraulic conductivity, θ is actual, θ_r residual, and θ_s saturated soil water content (L^3 L^{-3}). The equation differs in power (n) where Irmay used a value of 3 and Averkjanov 3.5. This simple equation may be less accurate than algorithms which describe K to h relationships, however, it may provide a simple means of limiting water movement to improve soil water content estimates in cascade models. Pressure head is sometimes not estimated in cascade models. Another option could be to use a pedo-transfer function such as employed in the SPAW soil water characteristics sub-model (Saxton and Rawls, 2006) to estimate soil water retention characteristics including unsaturated hydraulic conductivity as a function of soil water content and potential.

2.3.2 Modelling tile drainage

2.3.2.1 Steady state Hooghoudt equation

The steady state Hooghoudt equation is used in RZWQM2 and DRAINMOD to simulate tile drainage. The drawdown of water table height is not fully steady state, however, the rate of change usually proceeds slow enough that the Hooghoudt equation can be used effectively (Skaggs et al., 2012). The Hooghoudt equation as written in Skaggs et al. (2012) is;

$$q = \frac{4K_e m(2d_e+m)}{L^2} \tag{2.12}$$

where q (LT^{-1}) is the drainage discharge rate, K_e (LT^{-1}) is the effective lateral hydraulic conductivity, m is the water table level above the drain at midpoint between the drains, d_e is the equivalent depth of the impermeable (or restrictive) layer below the drain, and L is the drain spacing (Fig. 2.4a).

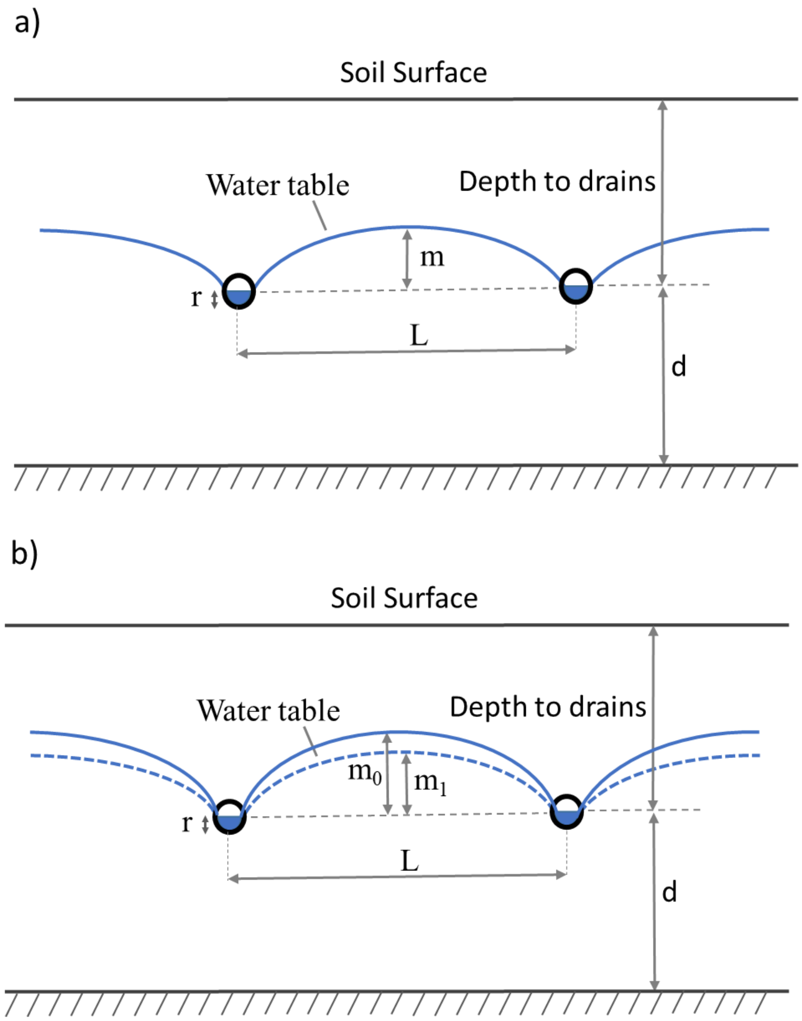

Figure 2.4 Drainage systems for a) steady state and b) transient conditions. L is the drain spacing, d is the depth from drains to the impermeable layer, r is the drain radius, and m, m_0, m_1 are the water table levels above the drain at midpoint between the drains for steady state (m), and before (m_0) and after drainage (m_1) for transient drainage.

Equations to estimate K_e and d_e below were outlined in Xian et al. (2017).

$$K_e = \frac{\int_{i=1}^{i=n} D_i K_i}{\int_{i=1}^{i=n} D_i} \tag{2.13}$$

where n is the number of soil layers, D_i is the thickness of layer i (L), and K_i is the lateral hydraulic conductivity of layer i (L T^{-1}).

The calculation of de depends on the actual depth (d; L) of the soil profile:

$$\text{if} \quad \frac{d}{L} < 0.3 \qquad d_e = \frac{d}{1+\frac{d}{L}\left[\left(\frac{8}{\pi} ln\frac{d}{r}\right) - CON\right]} \tag{2.14}$$

$$\text{where} \quad CON = 3.55 - 1.6\frac{d}{L} + 2\left(\frac{d}{L}\right)^2 \tag{2.15}$$

$$\text{if} \quad \frac{d}{L} \geq 0.3 \qquad d_e = \frac{L}{\left(\frac{8}{\pi} ln\frac{L}{r}\right) - 1.15} \tag{2.16}$$

where r is the radius of the drain (L).

2.3.2.2 Tile drainage under transient conditions

It is also feasible to calculate drainage based on a transient state approach whereby the water table height before and after drainage is taken into account (Fig. 2.4b). A recent study by Xian et al. (2017), when assessing the performance of RZWQM2 compared the steady state Hooghoudt equation and two transient equations including the Schilfgaarde equation (van Schilfgaarde, 1963; Bouwer and van Schilfgaarde,1963) and an alternative solution which allowed for use of the equation under larger time increments (van Schilfgaarde, 1964). The first equation proposed by van Schilfgaarde is written as;

$$L = 3A\sqrt{\left[\frac{K_e(d_e+m_1)(d_e+m_0)t}{2f(m_0-m_1)}\right]} \tag{2.17}$$

where

$$A = \sqrt{\left[1 - \left(\frac{d_e}{d_e+m_0}\right)^2\right]} \tag{2.18}$$

where m_0 and m_1 (L) are the water table levels above the drain at midpoint between the drains before and after drainage, respectively. T is the time period (T) and f is the drainable porosity (L^3 L^{-3}) which can be calculated as (Ma et al., 2007b): f = water content at saturation minus water content at field capacity.

The "integrated Hooghoudt equation" which allows for calculation at a larger time increment was derived by combining the Hooghoudt equation with mass balance equations (van Schilfgaarde, 1964) and it can be written as follows:

$$L = \sqrt{\frac{9K_e t d_e}{f ln[\frac{m_0(2d_e+m_1)}{m_1(2d_e+m_0)}]}} \tag{2.19}$$

The final water table height and the resulting change in water table height (Δh = m0 – m1) can be estimated as:

$$m = \frac{2d_e m_0}{2d_e e^Z + m_0 e^Z + m_0} \tag{2.20}$$

$$\text{where } Z = \frac{9Ktd_e}{fL^2} \tag{2.21}$$

The drainage coefficient or drain out flow can then be estimated by:

$$D_C = f * \Delta h \tag{2.22}$$

2.3.3 Water uptake via roots

Temperature is considered to be the main driver for root growth (Kage et al., 2000; Thorup-Kristensen, 2006; Kirkegaard and Lilley, 2007) which is often calculated based on cumulative day-degrees (CDD) defined as follows:

$$CDD = \begin{cases} 0 & ; T_{min} \geq T_{max} \\ T_{air} - T_{min} & ; T_{min} \leq T_{air} < T_{max} \\ T_{max} - T_{min} & ; T_{air} \geq T_{max} \end{cases} \tag{2.23}$$

Pedersen et al. (2010) suggested the following equation for estimating root penetration depth (R_z) expressed in terms of CDD;

$$R_z = \begin{cases} R_{zmin} & ; CDD \leq CDD_{lag} \\ \sum\left(\left(CDD - CDD_{lag}\right)k_{rz}\right) + R_{zmin} & ; CDD > CDD_{lag} \\ R_{zmax} & ; CDD - CDD_{lag}k_{rz} + R_{zmin} > R_{zmax} \end{cases} \qquad (2.24)$$

where R_z is the depth of root penetration; R_{zmin} is the planting depth; CDD_{lag} accounts for the time period between planting and start of root penetration (germination); k_{rz} is the root depth penetration rate with values provided for some crops in Pedersen et al. (2010); R_{zmax} is the maximum root penetration depth which can be determined based on several published studies (Fan et al., 2016; Benjamin et al., 2013). Note that equation 2.24 does not consider the impact of soil properties on root growth and development thus the maximum rooting depth set for a crop should take this into account.

A simple algorithm for root distribution, which was primarily based on a study by Gerwitz and Page (1974) was modified by Yang et al. (2009) to extend the rooting depth of fine roots by an additional 30%. This can account for very fine root biomass which is difficult to measure, but can also perhaps partially emulate capillary rise in models which are limited to cascade (tipping bucket) water flow. In equation 2.25 the root density declines logarithmically to the root penetration depth (R_z) followed by a linear decrease to zero at $1.3R_z$. The relative root length distribution is as follows;

$$L_R(z) = \begin{cases} e^{-a_z z} & ;\ z < R_z \\ e^{-a_z z}\left(1 - \frac{z - R_z}{0.3R_z}\right) & ;\ R_z \leq z \leq 1.3R_z \end{cases} \qquad (2.25)$$

where a_z is the shape parameter describing root distribution with increasing soil depth. Pedersen et al. (2010) used values of a_z = 2 for wheat and winter wheat and 1.5 for brassicas. The shape parameter and rooting depth can be defined based on field studies or from sources such as Fan et al. (2016) and Benjamin et al. (2013). Also, Pedersen et al. (2010) compared the exponential-based root distributions determined by equation 2.25 to observed data and found that it did well for monocots, but not always for dicot crop species. In general, Pedersen et al. (2010) found that equations 2.24 and 2.25 improved the simulation of both soil water and N in the profile.

Connecting text to Chapter 3

Chapter 2 provides a review of the DNDC model including a brief history of model developments and weaknesses of the soil hydrology algorithms. An overview of the hydrologic routines used in RZWQM and a general review of soil hydrologic processes, ranging in complexity, are also included. This sets the background for Chapter 3 where detailed comparisons of DNDC and RZWQM were made to determine which soil hydrologic processes in DNDC should be targeted for improvement. Both models were similarly calibrated and validated using observed measurements of crop yield, biomass, crop N uptake, soil water content, daily tile drainage and N loading from a 5 year maize-soybean rotation with and without a cover crop. It was deemed important to assess the entire water balance and impacts on N losses and crop growth since imperfections in water simulation cascades throughout the entire agroecosystem.

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Chapter 3

Comparing hydrological frameworks for simulating crop biomass, water and nitrogen dynamics in a tile drained soybean-corn system: Cascade vs computational approach

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Abstract

Biophysical agricultural models are needed for assessing science-based mitigation options to improve the efficiency and sustainability of agricultural cropping systems. It is crucial that they can accurately simulate soil hydrology and nutrient flows which strongly influence crop growth, biogeochemical processes and water quality. The purpose of this study was to compare the performance of the DeNitrification DeComposition model (DNDC), which utilizes simplified hydrologic processes, to a more comprehensive water flow model, the Root Zone Water Quality Model (RZWQM2), to determine which processes are sufficient for simulating water and nitrogen dynamics and recommend improvements. Both models were calibrated and validated for simulating soil hydrology, nitrogen loss to tile drains and crop biomass using detailed observations from a corn (*Zea mays L.*) -soybean (*Glycine max (L.) Merr.*) rotation in Iowa, with and without cover crops. DNDC performed adequately across a wide range of metrics in comparison to a more hydrologically complex model. Soybean and corn yield, and corn biomass over the growing season were well simulated by both models (NRMSE<25%). Soybean yields were also very well simulated by both models (NRMSE<20%); however, soybean biomass was over-predicted by RZWQM2 in the validation treatments. The magnitude of winter rye biomass and N uptake was well simulated but the timing of growth initiation in the spring was inaccurate at times. The annual and monthly estimation of tile flow and nitrogen loss to tiles drains were well simulated by both models; however, RZWQM2 performed better for simulating soil water content, and the dynamics of daily water flow to tile drains (DNDC: NSE -0.32 to 0.24; RZWQM2: NSE 0.35 to 0.69). DNDC overestimated soil water content near the soil surface and underestimated it in the deeper profile. We recommend that developments be carried out for DNDC to include improved root density and penetration functions, a heterogeneous and deeper soil profile, a fluctuating water table and mechanistic tile drainage. However, the inclusion of

computationally intensive process needs to be assessed in the context of improved accuracy weighed against the model's broad applicability.

3.1 Introduction

The performance of beneficial management practices for reducing nutrient losses from agricultural systems can vary both temporally and spatially in response to climate variations and soil diversity in the landscape. Process-based agricultural models can be valuable tools for extrapolating impacts of management over space and time. It is well known that many of the connected crop-soil-atmospheric processes are strongly influenced by water, and thus the performance of these models is highly correlated with how these hydrological processes are defined. Most models are developed to quantify a specific outcome such as crop biomass, greenhouse gas emissions, soil carbon change, or water quality and as a result the ability of the model to simulate hydrology is often simplified. The design philosophy that developers often choose is one which leans towards utilizing more simplified processes in order to keep the user expertise, input requirements, model transparency and computation time manageable. It is important for modellers to understand the limitations imposed by the hydrological modelling framework such that informed decisions can be made regarding the range of applicability and outcome quality.

The DNDC model is one of the most widely used process-based models for agriculture, and is arguably the most sophisticated for estimating greenhouse gas emissions; however, the model simulates simple cascade water flow and does not include a mechanistic drainage sub-model. In a recent review of C&N models, DNDC was found to be the only model which estimated all C&N related GHG emissions considered (Brilli et al., 2017), however, the model demonstrated weaknesses in simulating soil hydrology and the overall water budget and requires improvement (He et al., 2018b; Brilli et al., 2017; Congreves et al., 2016b; Dutta et al., 2016b; Uzoma et al., 2015; Smith et al., 2008; Cui et al., 2014; Abdalla et al., 2011; Deng et al., 2011). DNDC has been employed to estimate water drainage and NO_3-N loading in the U.S (Gopalakrishnan et al., 2012; David et al., 2009; Tonitto et al., 2007a, 2007b, 2010; Li et al., 2006) and China (Li et al., 2014; Zhao et al., 2014) and once calibrated the model generally performed well, however, the model was not tested systematically for simulating crop biomass, soil water content, and daily water flow in these studies. Recent studies have shown that DNDC outperformed other water budget models (Guest et al., 2018) largely because it includes a crop growth sub-model which integrates daily crop growth, water, nitrogen and heat stresses. DNDC performed similarly to cascade models DayCent and STICS for simulating soil water content but performed better for simulating soil N, particularly over STICS, which at the time did not include a soil freeze-thaw sub-model. STICS overestimated N loss in the late fall but snow insulation and freeze-thaw have now been incorporated (summer 2018). DNDC has not been benchmarked against a computational-based water quality model for assessing full system water and N dynamics.

The USDA-ARS Root Zone Water Quality Model (RZWQM2; Ma et al., 2012) is a detailed hydrologic model for simulating biogeochemical processes in the root zone. The model, released in 1992, includes design features and concepts from several other root zone models. The Decision Support System for Agrotechnology Transfer (DSSAT; Hogenboom et al., 2017) crop model is also embedded in its code. The benefit of using DSSAT is that it is widely used for simulating crop growth and phenology worldwide. The RZWQM2 model simulates a wide range of soil-plant-atmospheric processes and includes much more detailed hydrologic processes than DNDC including the Green-Ampt equation for infiltration, Richards equation for water flow, and Hooghoudt's equation for tile drainage. Several studies have shown that RZWQM2 can be employed successfully for simulating water flow to tile drains (Xian et al., 2017; Ma et al., 2012; Qi et al., 2011b; Akhand et al., 2003; Kanwar et al., 1997).

There have previously been successful comparisons of crop models which use simpler hydrology to computational models (Malone et al., 2017) but such assessments are rare, particularly across a wide range of metrics at high temporal resolution. In order to properly understand and quantify model performance, detailed input data and a wide array of observations for benchmarking water, soil and crop related processes are crucial. In this paper we use a comprehensive dataset that includes measurements of corn and soybean yields (common crops grown in the Midwestern U.S), corn, soybean and winter-rye biomass, crop N uptake, continuous soil water content at multiple depths, and near continuous estimates of water flow and N loading to tile drains across multiple years (Qi et al., 2011a, b; Ma et al., 2012). The objectives of this study were to i) calibrate and validate the DNDC and RZWQM2 models for simulating crop growth, soil water flow and nitrogen loading to tile drains in cropping systems with and without cover crops; ii) compare the performance of the models for simulating crop growth, soil hydrology and water quality and iii) document the strengths and weaknesses of the models for simulating water flow and N loss to tile drains and recommend future developments. In doing so we compare the performance of simpler water processes in DNDC, which are in fact common in many agricultural models, to the more detailed hydrology-based model, RZWQM2, in an effort to discern what level of process complexity is necessary for simulating water quality at daily, monthly and annual scales.

3.2 Materials and methods

3.2.1 Field studies

The model comparison was performed using measurements of water flow, N loss to tile drains, and biomass data from a corn-soybean study with and without cover crops at the Agricultural Drainage Water Quality - Research and Demonstration Site near Gilmore City in Pocahontas County, north central Iowa (42°42'N 104°00'W) (Lawlor et al., 2008; Qi et al., 2011a,b). The general soil texture classification of the site is a fine-loamy or fine clay loam and included 4 soil classifications; Nicollet, Webster, Canisteo, and Okoboji (USDA, 1985). The average particle size distribution near the soil surface across the 16 plots used in our analysis was 32% sand, 34% silt and 32% clay and the bulk density was 1.37 g cm^{-3}. The average annual (Jan 1st to Dec 31st) temperature was 8 ^{o}C and annual precipitation was 821 mm.

As part of a larger study 16 hydrologically distinct plots (15 x 38 m long) of completely randomized block design were established in the fall of 2004 and lasted 5 years until 2009. The study consisted of two treatments with cover crops and two controls, each with 4 reps. Treatment 1 (TRT1) consisted of winter rye prior to corn in odd years and prior to soybean in even years whereas treatment 2 (TRT2) was the reverse phase with winter rye prior to soybean in odd years and prior to corn in even years (Table 3.1). The controls (CTRL1 and CTRL2) included the same cropping system, but with no winter rye cover crop. Rye (*Secale cereale*; brand name: Rymin'; 3,638,000 seed ha^{-1}; 19 cm row spacing), Glyphosate-resistant corn (Dekalb 50-45; 77,000 seed ha^{-1}; 76 cm row spacing) and soybean (Pioneer 92M40 Group 2 middle season; 439,750 seed ha^{-1}; 76 cm row spacing) were planted using a drill seeder with dates determined by field conditions but at the same dates for control and no-control treatments. The agronomic practices for tillage and fertilizer application were consistent with those usually employed in Iowa and the scheduling of events is shown in Table 3.1. Aqueous ammonia fertilizer at a rate of 140 kg N ha^{-}

^{1} was applied on corn shortly after emergence and no fertilizer was applied to the soybean or winter rye. Tile drains were 106 cm deep, 7.6 cm diameter, and drain spacing was 7.6 m.

The Gilmore City site included a large complement of measurements such as water content at 4 depths, biomass and crop N uptake and daily time step measurements of water flow and N concentration to tile drains. From 2006 to 2009 corn and soybean biomass were sampled once every 3 weeks at 4 random locations in each plot until October and rye roots were sampled weekly. The combustion method was used for analyzing total nitrogen content of tissue samples. Corn and soybean yields were determined by combining 12 of 20 rows and grain seed was weighed for each combine pass.

Soil water content was determined using calibrated permittivity measurements from a Theta probe (Delta-T Devices) and a PR2 profile probe. Equations from Kaleita et al. (2005) were used to convert the permittivity values from the Theta probe to volumetric soil water content and water contents determined from *in-situ* soil measurements were used to calibrate the PR2 probe. In each plot permittivity was measured at 2 locations using the Theta probe for the 0-5 cm depth. The PR2 probe was used to measure permittivity at 0–10, 10–20, 20–30, 30–40, 50–60 and 90–100 cm profile depths via a fiberglass access tube. Measurements were taken on a weekly basis from March through October, 2006–2008.

The water loss from the subsurface tile drains was measured using a flow meter and prior to 2006 the volume was manually recorded on a weekly or bi-weekly basis. After April 2006 a magnetic recorder was used allowing for measurements at 0.005 cm water depth intervals (increments of 14 L). Samples of drainage flow were collected approximately every 1.3 cm of drainage flow and stored at 4^{o}C for analysis. The second-derivative spectroscopy technique was used to analyze NO_3-N concentration which was multiplied by the drainage volume to calculate NO_3-N loss from the tile drains. For details regarding sampling techniques see Qi et al. (2011a, c) and Lawlor et al. (2008).

Table 3.1 Cropping systems and agronomic practices at the Gilmore City site, Iowa from 2005 to 2009

	2005	2006	2007	2008	2009
Treatment					
TRT1, Calibration	rye-corn	rye-soy.	rye-corn	rye-soy.	rye-corn
CTRL1, Validation	corn	soybean	corn	soybean	corn
TRT2, Validation	rye-soy.	rye-corn	rye-soy.	rye-corn	rye-soy.
CTRL2, Validation	soybean	corn	soybean	corn	soybean
Management activity					
Termination of rye prior to corn	April 30	April 24	April 30	May 6	May 8
Cultivation[(a)] and corn planting	May 10	May 4	May 14	May 15	May 19
Cultivation[(a)] and soybean planting[(b)]	May 18	May 10	May 17	May 23	May 20
Termination of rye	May 20	May 16	May 23	May 26	May 31
Fertilize corn (140 kg N ha^{-1})	May 25	May 18	June 5	June 4	June 30
Corn and soybean harvest	Oct. 10	Oct. 7	Oct. 22	Oct. 20	Nov. 3
Chisel plow (CTRL1, 2)	Oct. 10	Oct. 10	Oct. 24	Oct. 20	no-till (wet)
Disk plow and cultivation (TRT1, 2)	Oct. 10	Oct. 10	Oct. 24	Oct. 20	no-till (wet)
Plant rye	Oct. 11	Oct. 12	Oct. 25	Oct. 21	Nov. 20

a) Only CTRL1 and CLTRL2 were cultivated
b) DNDC handles intercropping but not RZQWM2, thus for RTWQM2 soybean was planted after rye termination

3.2.2 Model overview

As discussed in the following sections the DNDC model employs simple equations and methods for soil hydrology whereas RZWQM2 which was primarily developed for simulating water quality thus includes much more mechanistic and computation intensive equations (Table 3.2, Fig. 3.1). An earlier version (2.0 2010) of the RZWQM2 was previously calibrated and validated for the Gilmore City site (Qi et al., 2011b) but in this study a newer version (3.0 2015) was employed in a similar manner using calibration and validation procedures described in Ma et al. (2012). Once calibrated the newer version performed similarly with marginally improved results.

3.2.2.1 DNDC

The DeNitrification DeComposition (DNDC) model (Li et al., 2012) is a widely used process-based model for simulating the effects of climate and agricultural management on crop growth, soil C&N cycling, trace gas emissions, and nutrient loss from runoff and drainage. It includes several sub-models for predicting crop growth, soil climate, decomposition, nitrification, denitrification, and fermentation. The model was first developed to estimate nitrous oxide emissions, but was later expanded to estimate soil C&N cycling, water drainage and nitrogen loss to tile drains (Li et al., 2006) and finally to include full farm facility and livestock systems (Li et al., 2012). The model has been tested and validated extensively for simulating crop growth, GHG emissions, soil carbon change, and ammonia volatilization worldwide (Ehrhardt et al., 2018; Brilli et al., 2017; Zhang and Niu, 2016; Gilhespy et al., 2014) but it has seldom been tested for simulating water flow and nutrient losses to tile drains.

Efforts are made by the model developers to minimize the amount of input data and process time required thus some of the processes in DNDC are purposefully kept simple. The current release version of DNDC employs a cascade flow water model simulating bulk water flux and N transport through the profile (Table 3.2, Fig. 3.1). Nitrate movement in DNDC was conceived as a function of the water flux per layer. Soil NO_3^- is considered to be mobilized by positive water flux (90% mobilized) and transferred to the layer below as a one-dimensional vertical N flux towards the bottom soil profile. The movement of NO_3^- is an iterative step through each of the saturated layers per hour. Additionally, another fraction (10% of the NO_3^- in each layer) is considered to be lost through preferential water flow via macropores directly out of the soil profile. Nitrate fertilizers are added directly to the soil NO_3^- pool thus they may be more subject to more initial leaching. Urea is moderately mobile in the model whereas NH_4^+ is not mobile. Ammonium-based fertilizers undergo nitrification to NO_3^- before movement can occur and urea undergoes hydrolysis to NH_4^+ followed by nitrification to NO_3^- (Dutta et al., 2016a). Nitrate travels through the profile in solution, and is leached from the 50 cm depth. This is the value that is considered to be lost to tile drains, regardless of the depth of the actual drains.

Li et al. (2006) included a “deep water pool” to increase the default 50 cm soil profile depth to that of a tile drain; however, the deep water pool depth (default 50 cm) can’t be adjusted without recompiling the model, N adsorption and transformations are not included in the additional profile, and a fluctuating water table is not simulated. Water which leaches from the 50 cm depth moves into the deep water pool. Water which leaches from this pool is considered to be lost to tile drains. Adsorption and desorption of NH_4^+ based on the Langmuir equation was also incorporated in his study (top 50 cm of soil profile) as well as a simplistic empirical relationship or “recession curve” to delay drainage by soil layer. This recession curve required parameterization of coefficients for each soil type (Tonitto et al., 2007a), and is no longer active in the current release version. Tonitto et al. (2007a,b) found that after calibration of the recession equation in DNDC the model performance was satisfactory for simulating annual water flow and nitrate loss to tile drains when aggregated across a watershed; however, DNDC consistently under-predicted monthly drainage and the model was not tested using daily data.

Several modelling teams have developed specific versions of the model to better enable the simulation of regional soils, climate events, crop cultivars and management practices. In our study, a Canadian version of DNDC (DNDCv.CAN) was employed which is well suited for over-winter conditions that occur in Iowa. This version was developed over the last several years by introducing crop specific growth curves for wheat, corn and soybean (Grant et al., 2016) and by improving the prediction of evapotranspiration (ET) (Dutta et al., 2016b). Transpiration is based on the crop water demand but is limited by soil water status. In the model transpiration is determined first, with a minimum of 10% potential evapotranspiration reserved for evaporation. Evaporation from the soil, leaves, and stem are then calculated as a function of the remaining PET. A new ammonia sub-model for simulating manure slurry and urea additions was incorporated (Congreves et al., 2015b; Dutta et al., 2016a). The model was also revised for simulating the effects of biomass, crop residue, snow cover, and soil texture on soil temperature (Dutta et al., 2018). At the beginning of this study all developments for Canada DNDC were added to the U.S. release version thus creating an up to date model version which includes both the U.S. and Canadian developments (available at https://github.com/BrianBGrant/DNDCv.CAN).

3.2.2.2 RZWQM2

The Root Zone Water Quality Model (version 3.0.2015; Ma et al., 2012) was developed to simulate major biogeochemical processes in agricultural systems that affect water quality in the plant root zone and below the root zone, runoff and to tile drains. The model is largely one-dimensional but includes quasi-two-dimensional lateral flow to tile drains. Similar to DNDC, the model simulates a wide range of agricultural management practices but it includes more detailed processes for simulating water and nutrient transport including mechanistic tile drainage (Table 3.2, Fig. 3.1). RZWQM2 includes DSSAT 4.0 Cropping System Models (Jones et al., 2003) with CERES and CROPGRO components (Ma et al., 2005, 2006) and thus can simulate crop growth and development for a wide range of crops using an established and verified framework. RZWQM2 is more data intensive than DNDC requiring a more detailed physical representation of the soil profile. It requires parameters for describing soil water retention and other hydraulic properties. It also requires more intensive computer processing time since it simulates a heterogeneous soil profile and includes mechanistic equations such as numerical procedures for solving the Richards equation and Green-Ampt infiltration (Table 3.2, Fig. 3.1). Our hypothesis is that RZWQM2 should be more accurate than DNDC in predicting water flow and nutrient loading but will require more data to initialize and calibrate.

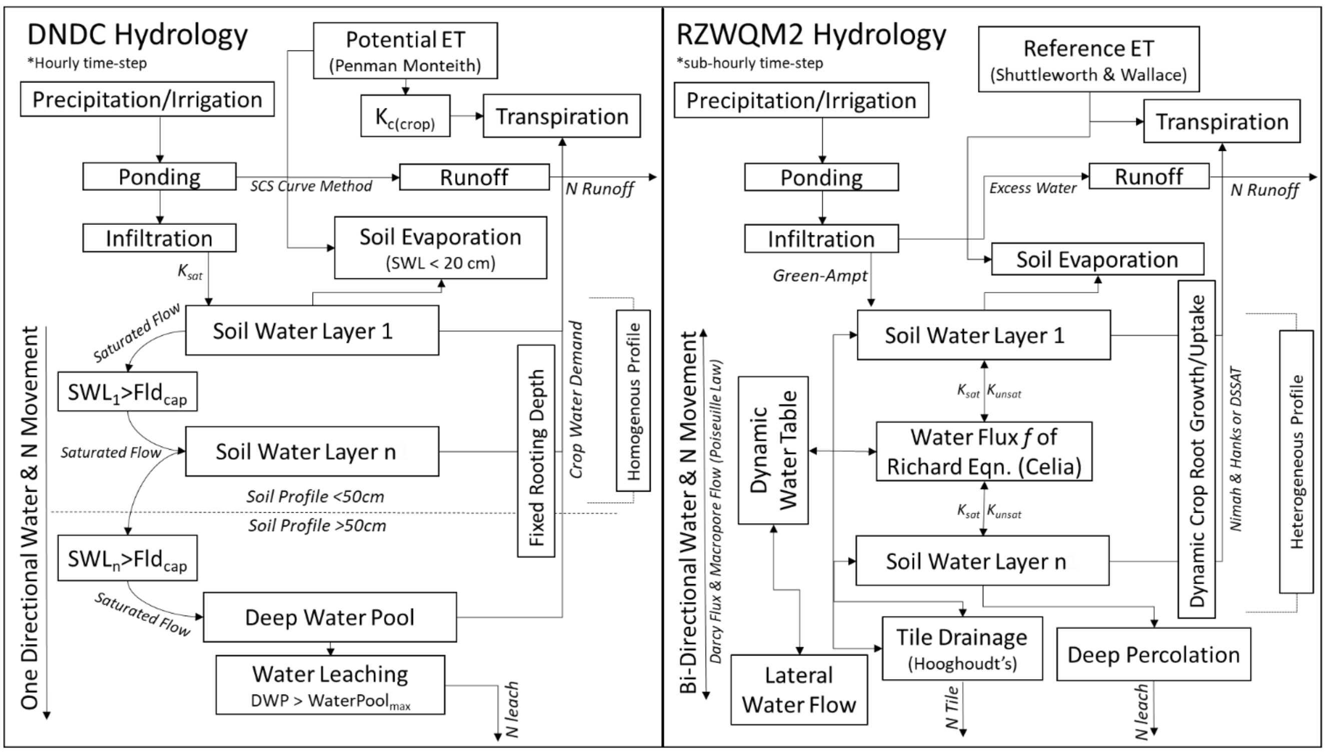

Figure 3.1 Schematic of hydrological processes in DNDC and RZWQM2

Table 3.2 Comparison of hydrological processes used in DNDC and RZWQM2

Hydrology component	DNDC	RZWQM2
Soil profile	Homogeneous soil properties to 50 cm depth, layers ~2 cm thickness, underlying deep water pool to 100 cm depth.	Heterogeneous soil properties, customizable soil profile to several meters depth
Soil water transport	Water drains between soil layers if above field capacity (cascade “tipping bucket” flow)	Water redistribution simulated by Richards Equation, Brooks Corey soil-water characteristics curve, macropore flow option
Infiltration and runoff	Runoff is removed based on the SCS curve number method, followed by canopy interception, then infiltration is limited by surface saturated hydraulic conductivity (K_{SAT})	Modified Green-Ampt approach to estimate infiltration rate, water excess goes first to macropores and then to runoff
Potential Evapotranspiration	Penman-Monteith FAO approach with coefficients for each crop type, transpiration is a function of PET and crop water uptake demand determined by biomass	Modified Shuttleworth-Wallace model, constrained by water availability, multiple crop water stress options, reduces evaporation under residue-covered soil
Tile drainage	Bulk gravity drainage with no deep seepage considered	Hooghoudt’s equation, adjustable tile drainage depth, tile diameter, and drain spacing
Water table	None simulated	Fluctuating water table

3.2.3 Model initialization, calibration and validation

For each research location, treatment 1 (includes a winter rye cover crop) was used to calibrate the models whereas treatment 2 and the controls were used to validate the models. Calibration was conducted by trial and error, in a stepwise manner by minimizing RMSE for yield, biomass, drainage and N loss to tiles. Model simulations were run for a ten year spin-up period prior to the beginning of the experiment to stabilize water and N pools in the models. Soil inputs including percent sand, silt and clay, bulk density, soil C content, field capacity and wilting point were available from measurements taken at the site across several depths (Table 3.S1). Soil properties were not measured below 120 cm, thus the values from the 90-120 cm depth were assumed to apply below 120 cm. Soil properties were similar between plots and initial tests with both models indicated little influence on modelled water dynamics, thus the same properties were used for all treatments and controls, similar to Qi et al. (2011b).

3.2.3.1 RZWQM2 calibration

Detailed soil properties were input for each measured depth increment (Table 3.S1). The initial carbon and nitrogen residues in the soil profile were determined from Thorp et al. (2007), including crop residue and microbial pools. Initial soil moisture was set based on sampling in November 2005 with saturation occurring below 60 cm depth to initiate the simulation of a water table in the model.

The soil depth above the impermeable layer was set to 390 cm and a K_{SAT} rate of 0.01 cm h^{-1} was set in the bottom layer to limit flow and maintain the water table. The lateral saturated conductivity used in the Hooghoudt equation, for each soil layer, was set to $2K_{SAT}$. The modified Brooks-Corey equation is a four parameter nonlinear curve fitting model for fitting water retention data (Ma et al., 2012). Two of these parameters, saturated and residual water contents, were based on one-third bar measurements. The other two parameters are used for curve fitting. The 2nd exponent of k-curve (N2) was calculated as $3\lambda + 2$, and the 2nd intercept (C2) was estimated as $Ksat \times P_b^{N2}$ where λ is the pore size distribution index and P_b is the bubbling pressure (cm). The background N in precipitation was set to 0.5 and 1.3 mg N L^{-1} for NH_4, and NO_3 respectively (Qi et al., 2011b).

Agriculture management practices including planting and harvest dates, tillage type and scheduling, fertilizer rates and scheduling were also used as inputs (Table 3.1). Most of the DSSAT crop parameters for the corn (IB 1068 Dekalb 521) and soybean (990002 M Group 2) were left as default (Table 3.S2); however, a few were modified to minimize NRMSE of yield in the calibration treatment (TRT1). For corn, three crop parameters were adjusted. The maximum possible number of kernels per plant (G2) and the kernel filling rate during linear grain filling stage (G3; mg d^{-1}) were decreased to 722 and 6.55, respectively. The phylochron interval between successive leaf tip appearance (PHINT: ^oC days) was increased to 46. For soybean only maximum leaf photosynthesis rate (at 30 C, 350vpm, and high light; LFMAX; umol CO_2 m^{-2} s^{-1}) was modified, lowering it from 1.03 to 0.80. The parameters of the winter rye crop were based on a U.S. winter wheat crop cultivar (990003 winter-US) since a winter rye cultivar was not available in the DSSAT database. Significant calibration was required with most of the calibration performed in Qi et al. (2011b). In this study we further adjusted four parameters to minimize NRMSE for biomass in TRT1 (Table 3.S2). Phylochron interval, time between successive leaf appearance (PHINT) was increased to 100, conversion rate from photosynthetically active radiation to dry mater before the end of leaf growth (PARUV; g MJ^{-1}) was increased to 3.3, lamina area to weight ratio of standard first leaf (LARWS; cm^2 g^{-1}) was increased to 300, and finally lamina area to weight ratio, phase 2 (LAWR2; cm^2 g^{-1}) was increased to 280. PHINT was adjusted to delay growth in the spring and the remaining three parameters were adjusted to increase growth rate.

Before calibration RZWQM2 simulated average annual mineralization rates that were lower than expected (~100 kg N $ha^{-1}y^{-1}$) which resulted in low rates of N loss to tile drains. Carpenter-Boggs et al. (2000) found that average mineralization rates were 142 kg N ha^{-1} for a 189 day growing season for a corn-soybean rotation in eastern South Dakota (clay loam soil at 1.8% soil C). RZWQM2 was calibrated by increasing the decay rates of the organic matter pools by ~38% which in turn resulted in an acceptable rate of N loss to tile drains (NARE -3.5%; NSE 0.92) and level of crop N uptake (NARE 6.4%; NRMSE 17%). Total organic N in the soil profile remained stable within 0.5% of the starting value over the five year study.

3.2.3.2 DNDC calibration

The DNDC model was less time consuming to calibrate largely because it employs less intensive hydrologic processes and equations with fewer parameters. The processing time for a simulation was 12 times faster. Only the soil physical and chemical properties for the top soil layer are required as input (Table 3.S1). These properties include bulk density, soil texture, clay fraction, field capacity at 0.33 bar, wilting point at 15 bar, pH, K_{SAT}, porosity, soil organic carbon. The model employs a pedo-transfer function to estimate a decline in soil carbon and an increase in bulk density down the soil profile. This may result in an erroneous approximation of the soil profile. The N concentration in precipitation was set to be 1.8 mg N L^{-1} to be equivalent to the total value used in RZWQM2. This resulted in an average annual atmospheric N input of 14.1 kg N $ha^{-1}y^{-1}$. DNDC uses the SCS runoff curve number method developed by the USDA Natural Resources Conservation Service and also the Modified Universal Soil Loss Equation (MUSLE) which includes the Manning's coefficient for overland flow. For runoff, the SCS curve number was set to 64 for a well-drained row crop with residue and clay loam soil and the Manning's roughness coefficient was set to 0.19 for conventional tillage with residue. The option was employed to use all climate drivers on a daily time step (maximum and minimum temperature, precipitation, wind speed, radiation and relative humidity).

DNDC requires similar agricultural management inputs as RZWQM2 (Table 3.1). The crop parameters in DNDC are simpler and less varied; however, they often require substantial modification since values are generalized for specific crop types and are not provided for cultivars. The user inputs are easily understood and include inputs such as “max biomass production of grain”, biomass fractions of plant organs, C:N ratios of plant organs, thermal degree days to maturity, water demand (g water/g dry matter), and optimum temperature for growth. Other crop parameters are internal per crop type and cannot be modified without recompiling the model, such as minimum and maximum temperature for growth, effect of atmospheric CO_2 on assimilation, effect of CO_2 on water and N use efficiency, and temperature stress during anthesis. In this study we modified the default parameters for corn, soybean and winter wheat to minimize NRMSE for yield. The thermal degree days to maturity (TDD) for soybean was set to 2500, the crop water demand was increased from 350 to 420 g water/g dry matter and max (potential) biomass of grain was set to 2550 kg C $ha^{-1}y^{-1}$. For corn the max biomass of grain was set to 4500 kg C $ha^{-1}y^{-1}$ and the C:N ratios of grain, leaf and root were modified from 50, 80, 80 to 35, 70, 70, respectively, to increase and improve N uptake relative to average measured values, and resulting N stress affecting corn yields/biomass. The default rye crop in DNDC was adjusted to improve the simulation of winter rye biomass relative to the control by lowering the TDD from 2000 to 1400, and lowering the optimum temperature for growth from 25 to 18 ^oC.

Similar to RZWQM2 the default SOC partitioning, SOM pool sizes, and decay rates resulted in too little N mineralization and under prediction of N in tile drains. The humus fraction was lowered from 0.8 to 0.7. After calibration the average annual mineralization over the five year study was simulated to be 169 kg N $ha^{-1}y^{-1}$ in RZWQM2 whereas it was 170 in DNDC.

3.2.4 Statistical measures for testing model performance

The following statistical measures were used to evaluate model accuracy in predicting crop yields, biomass and crop N: Pearson’s r correlation coefficient (r), normalized average relative error (NARE; %) and normalized root mean square error (NRMSE; %). The NARE value represents the percent over- or under-prediction of a model relative to measurements. It is similar to precedent bias (PBIAS) but of opposite sign.

$$r^2 = \left(\frac{\sum_{i=1}^{n}(O_i-\bar{O})\times(P_i-\bar{P})}{\sqrt{\sum_{i=1}^{n}(P_i-\bar{P})^2}\times\sqrt{\sum_{i=1}^{n}(O_i-\bar{O})^2}} \right)^2 \qquad (3.1)$$

$$NARE = 100\left(\frac{\frac{1}{n}\sum_{i=1}^{n}(P_i - O_i)}{\bar{O}}\right) \tag{3.2}$$

$$NRMSE = 100\left(\frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(O_i - P_i)^2}}{\bar{O}}\right) \tag{3.3}$$

$$NSE = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \tag{3.4}$$

where P_i is a predicted or simulated value, O_i is the observed value.

The Nash-Sutcliffe model efficiency coefficient (NSE) was applied for evaluating model performance in simulating soil hydrology and nitrate fluxes to tile drains. A value of greater than 0 for NSE (maximum possible value is 1) indicates the model estimates are more accurate than the average of observations.

Ahuja et al. (2000) considered model performance was satisfactory for yields and biomass if NARE<15% and Jamieson et al. (1991) considered excellent performance if RSME%<10; good<20; fair<30; and poor>30. Moriasi et al. (2007) suggested that model performance for simulating water and N flow was satisfactory if NSE>0.5, water flow if NARE<25% and N loss if NARE<70%.

3.3 Results and discussion

The Gilmore City dataset offers a large range of biomass, soil water storage, N and water flow measurements from daily to annual scales, which was systematically used to assess model performance and potential areas for improving hydrological processes in the following sections.

3.3.1 Crop yield and growth

Accurate simulation of crop growth including the impacts of temperature, water and nutrient stresses on production, is crucial for simulating water and N dynamics in agricultural models. Recently, Guest et al. (2018) reported that DNDCv.CAN outperformed two water budget models that do not simulate crop growth. In this study both DNDC and RZWQM2 performed well in simulating corn and soybean yields (Table 3.3; Fig. 3.S3a). RZWQM2 performed a little better than DNDC for corn across the three validation treatments but for both models NARE was <4% and NRMSE was < 11%. Soybean yields were slightly overestimated by both models (<8% NARE) and the NRMSE was higher than for corn but simulations were still considered to be "good". Higher relative NRMSE may be expected when simulating lower yields. RZWQM2 tested in this study performed marginally better (lower NARE and NRMSE) for both corn and soybean yields than did the 2010 version which was previously used to simulate the same cropping system (Qi et al., 2011b). The RMSE values for both DNDC and RZWQM2 in this study were lower for corn than in Jarecki et al. (2018) who estimated RMSE's of over 1100 kg DM ha^{-1} using DNDCv.CAN. The NRMSE for both models was, however, higher than estimated by He et al. (2018a) using DNDCv.CAN who calculated values from 4.0-6.1% for corn and 6.4-11.8% for soybean, but in each case the validation simulations were performed over only 2 years of data.

Table 3.3 Observed and simulated corn and soybean yields across the three validation treatments from 2005 to 2009 (kg DM ha^{-1})

	Corn			Soybean		
	Obs.	DNDC	RZWQM	Obs.	DNDC	RZWQM
Avg.	8800	8517	8723	2750	2914	2963
r^2		0.48	0.58		0.53	0.66
NARE		-3.2	-0.9		5.9	7.7
RMSE		892	831		477	403
NRMSE		10.1	9.4		17.3	14.7

Corn and soybean biomass over the growing season for the calibration treatment was predicted with "good" model performance by both RZWQM2 and DNDC (Table 3.4, Fig. 3.2). Note, however, that DNDC does not simulate soybean senescence which is a model weakness, likely resulting in an overestimation of the last biomass observation in 2008 (Fig. 3.2). DNDC also does not simulate water excess on crop growth as was pointed out in Sansoulet et al. (2014) but since this was a well-drained site there was likely little influence. Corn biomass was predicted with good performance by both models across all validation treatments with a little better performance by DNDC in TRT2 and CTRL2 (corn in 2006 and 2008).

Soybean biomass was predicted with "good" performance by both models for CTRL1. Observed soybean biomass was low in TRT2 and CTRL2 in 2007 and 2009 and DNDC captured this reasonably well (Fig. 3.2), however, RZWQM2 over-predicted biomass throughout most of the season. Note that simulated biomass decreased in RZWQM2 at the end of the season during senescence and the prediction of soybean yield for the validation treatments was "good" (Table

3.3). The models over-predicted biomass more so in TRT2 (Fig. 3.2) when observed soybean growth appeared to be supressed by low seasonal growing degree days (GDD) (Fig. 3.S1). The models were calibrated for soybean growth only in 2006 and 2008 when GDD was higher.

Table 3.4 Statistical performance of DNDC and RZWQM2 for simulating corn and soybean biomass. The study consisted of two treatments with cover crops and two controls. Treatment 1 (TRT1) consisted of winter rye prior to corn in odd years and prior to soybean in even years whereas treatment 2 (TRT2) was the reverse phase (Table 1). The controls (CTRL1 and CTRL2) included the same cropping system, but with no cover crop.

	------ Calibration -------			---------------------------------- Validation						--------------------------------------		
	Treatment 1			Control 1			Treatment 2			Control 2		
	Obs.	DNDC	RZWQM	Obs.	DNDC	RZWQM	Obs.	DNDC	RZWQM	Obs.	DNDC	RZWQM
Corn biomass (kg DM ha^{-1})												
Avg.	7251	7613	7360	7252	7340	7869	14060	12634	12819	13558	12864	12758
r^2		0.96	0.96		0.96	0.96		0.99	0.97		1.00	0.96
NARE		1.5	5.0		1.2	8.5		-8.8	-10.1		-5.9	-5.1
RMSE		1401	1356		1504	1357		1853	2824		1332	2264
NRMSE		19.3	18.7		20.7	18.7		13.2	20.1		9.8	16.7
Soybean biomass (kg DM ha^{-1})												
Avg.	3601	3806	3852	3741	3768	3856	1777	2101	2728	2185	2098	2737
r^2		0.95	0.90		0.90	0.93		0.96	0.96		0.88	0.95
NARE		5.7	7.0		0.7	3.1		18.3	53.6		-4.0	25.3
RMSE		665	689		800	540		751	1308		796	963
NRMSE		18.5	19.1		21.4	14.8		42.2	73.6		36.4	44.1

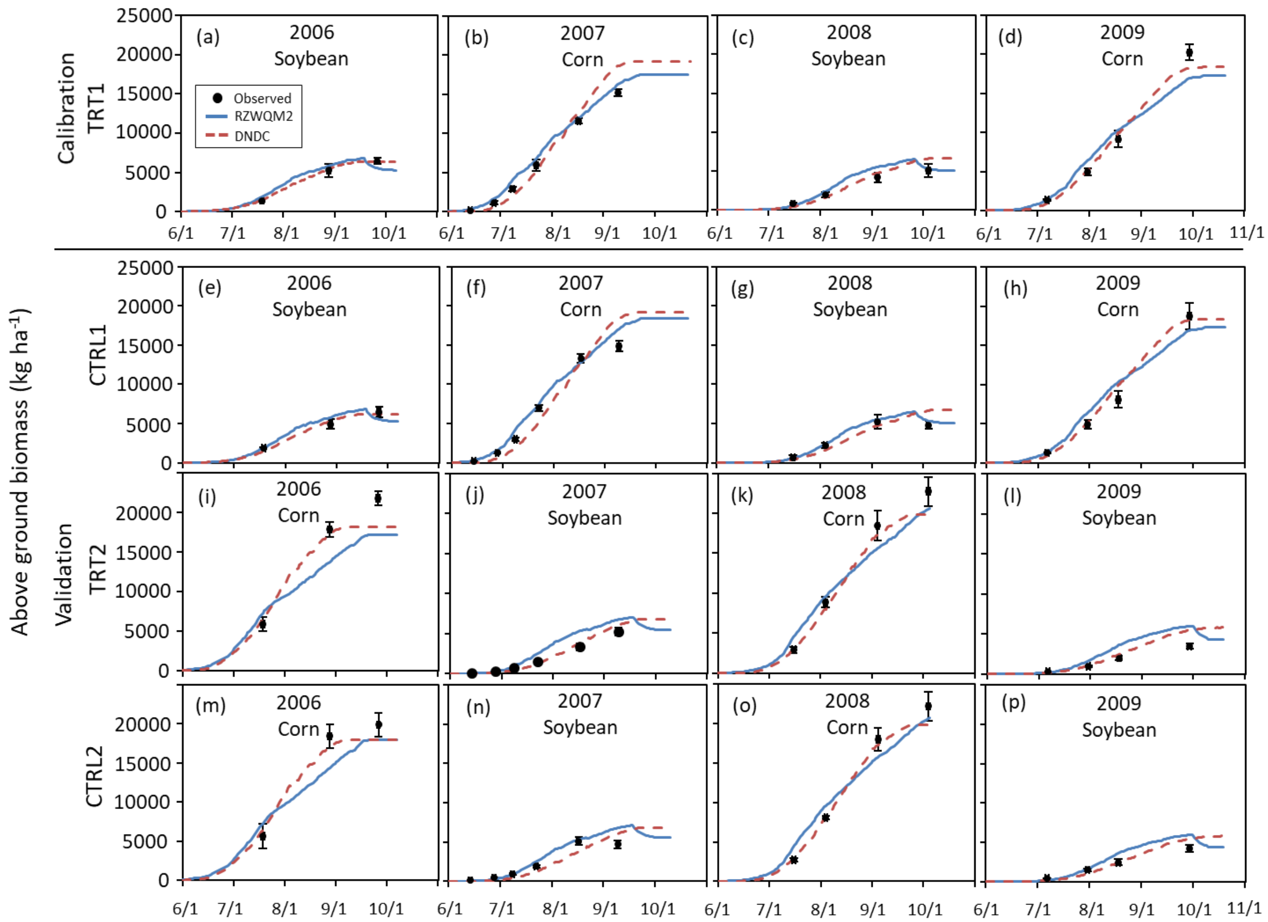

Figure 3.2 Observed and modelled corn and soybean dry biomass from 2006 to 2009 for calibration plot TRT1 (a-d) and validation plots CTRL1 (e-h), TRT2 (i-l), and CTRL2 (m-p)

The cumulative seasonal winter rye biomass and N uptake was predicted quite well by both models, with ARE always being less than 20%, however, the timing of growth and N uptake was sometimes off resulting in high NRMSE (Table 3.5, Fig. 3.S2). The high NRMSE was in part due to the low biomass and N uptake but there was also difficulty in simulating the correct timing of emergence in spring. In RZWQM2 a winter wheat cultivar was adjusted to simulate winter rye as no existing cultivar was available and in DNDC a “generalized” rye crop was adjusted to simulate winter rye. This suggests room for future improvement.

Table 3.5 Statistical performance of DNDC and RZWQM2 for simulating winter rye biomass and N uptake

	Treatment 1 - Calibration			Treatment 2 - validation		
	Obs.	DNDC	RZWQM	Obs.	DNDC	RZWQM2
Biomass (kg DM ha^{-1})						
Avg.	399	397	415	446	391	503
r^2		0.96	0.92		0.80	0.82
NARE		-.5	4.1		-12.4	12.9
RMSE		195	175		434	267
NRMSE		49.0	43.8		97.3	59.8
N uptake (kg N ha^{-1})						
Avg.	13.3	12.9	12.9	13.6	14.7	16.2
r^2		0.91	0.76		0.51	0.86
NARE		-2.8	-3.0		8.3	18.9
RMSE		4.9	7.5		13.7	9.3
NRMSE		36.6	56.7		100.8	68.5

3.3.2 Soil Hydrology

An analysis of water partitioning (Fig. 3.3) indicated that both models predicted similar levels of annual drainage, runoff and ET, with greater transpiration occurring in the years with cover crop, particularly for RZWQM2 which simulated on average 29.2 mm transpiration from winter rye in comparison to 19.2 mm for DNDC. It is interesting that the DNDC model which employs a simple cascade water flow approach predicted similar water balances as RZWQM2, particularly for treatments with no cover crop. There has, however, been considerable efforts recently to improve estimates of ET and adjust crop coefficients using the Penman-Monteith approach (Dutta et al., 2016b). ET is the largest component of water loss from the agroecosystem in this study and likely has a large influence on how much water is transported down the soil profile.

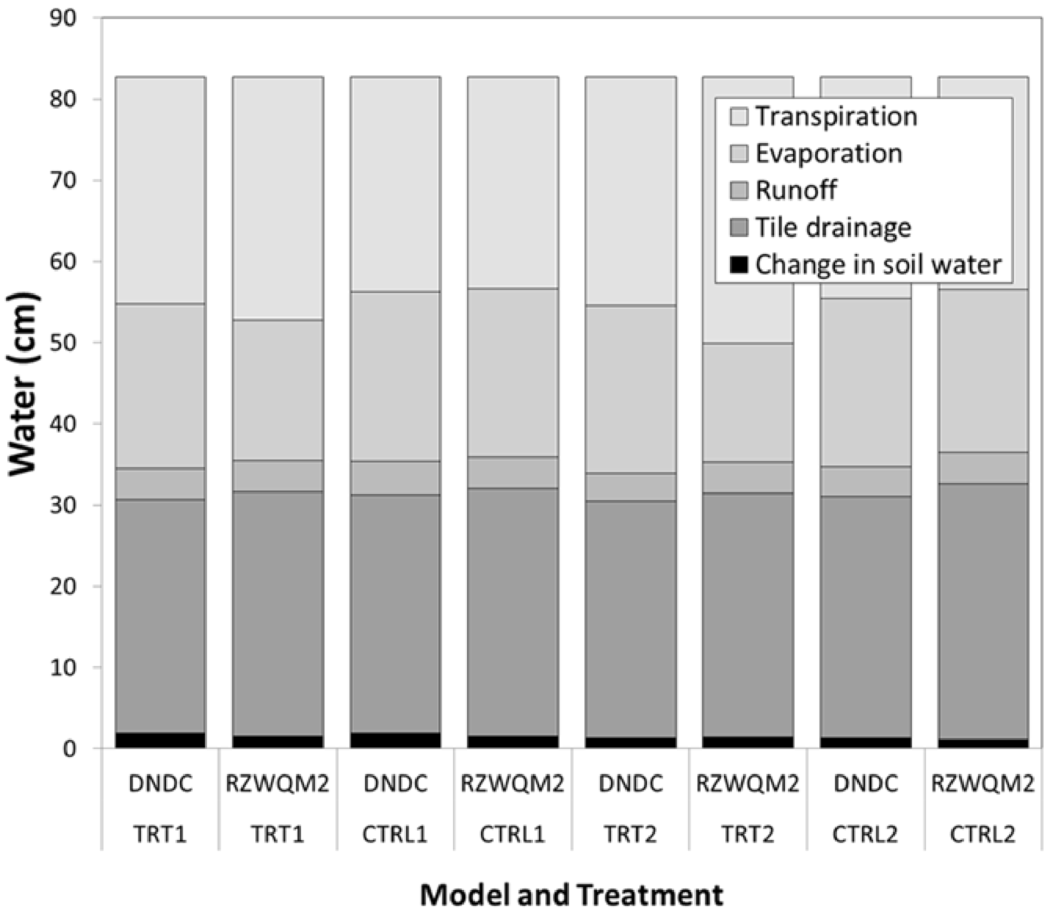

Figure 3.3 Simulated annual water budget (5 year average) using DNDC and RZWQM2

RZWQM2 performed much better than did DNDC for simulating soil water storage in the 0-60 cm soil profile (Fig. 3.4; Table 3.S3) and soil water content by layer (Fig. 3.S4). Since DNDC only simulates water to effectively 100 cm depth, and plant roots don't have access to the water table, soil water content during the warmer summer months were greatly underestimated in an attempt to meet crop demands. The inclusion of mechanistic tile drainage, allowing for simulation of a water table, would likely greatly improve water content simulation during the warmer periods. Soil water content was generally overestimated by DNDC near the soil surface and underestimated deeper in the profile which was presumably caused by the lack of root distribution algorithms, the inability to simulate a heterogeneous soil profile and no water table. The DNDC model currently does not estimate changes in root density in the soil profile and plants uptake water equally across the top 50 cm. It is expected that the inclusion of simple root density functions by crop type, such as those described by Pedersen et al. (2010), could further improve water uptake and the distribution of water down the profile. Note that DNDC currently only outputs soil water that is not frozen so the winter period is not shown. As reported in a recent review of C&N models (Brilli et al., 2017) and from other sources (He et al., 2018a; Dutta et al., 2016b; Uzoma et al., 2015; Abdalla et al., 2011; Deng et al., 2011; Smith et al., 2008; Saggar et al., 2004) DNDC was found to have weaknesses in simulating soil water content and in many of these studies the lack of the ability to simulate a heterogeneous soil profile was noted.

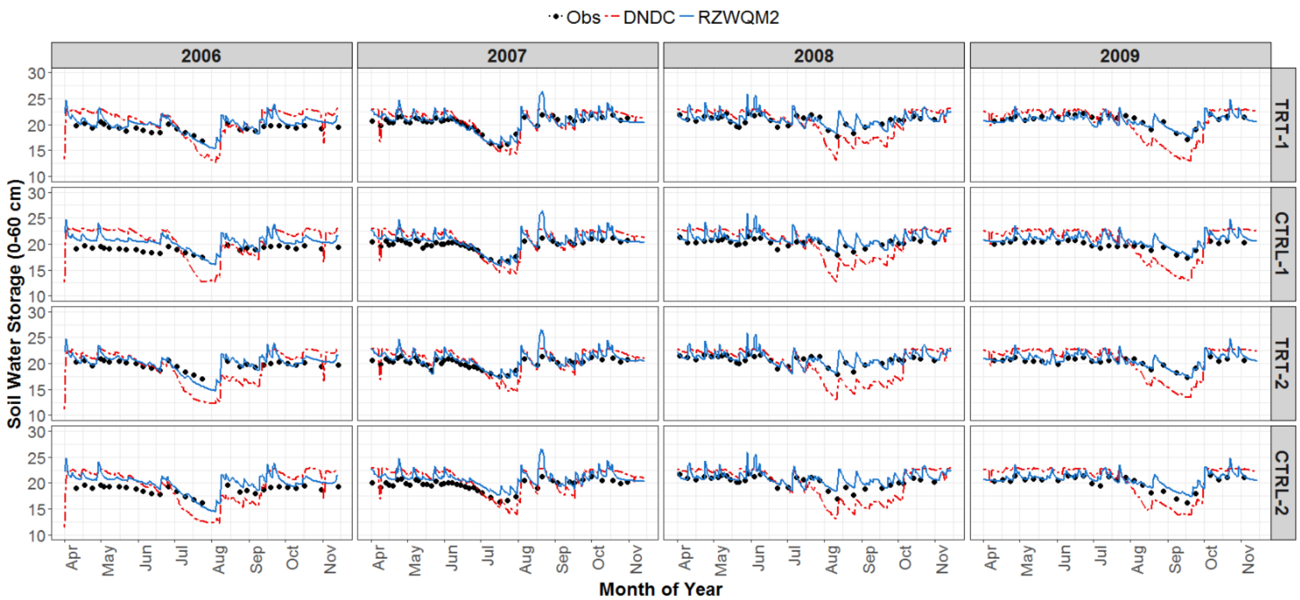

Figure 3.4 Observed and simulated soil water storage (0-60 cm).

3.3.3 Water flow and N loss to tile drains

The success of a model in simulating soil water and N dynamics is relevant to different time scales, determined by the criteria set forth in a study. Time scales of interest may include those over the growing season to estimate water and N dynamics for overall crop requirements or a shorter time frame may need to be considered to assess water and N during critical phases of growth. Further, it may be important to estimate N and P loss to drains and to runoff on a monthly basis in order to assess the risk of eutrophication in water bodies. On a daily basis soil water and N status is important for estimating several processes including N_2O emissions from denitrification which can be driven by individual rainfall events. Vergé et a l. (2017) found that the grey water footprint (volume of water required to dilute leached N concentration to 10 mg N L^{-1}) of corn production varied greatly across time scales, with the greatest footprint of 2700 mm water daily to zero annually. Thus in this study we assess water flow to tile drains at three different time steps, daily, monthly and annually. Nitrogen loss to tile drains is assessed monthly and annually since N concentration in bulk water samples was measured only when water attained a certain depth in the collecting reservoir (generally 1 to 2 weeks).

3.3.3.1 Water flow to tile drains

The DNDC model performed well for simulating water loss to tile drains on an annual basis from 2005 to 2009 with similar statistics to RZWQM2 (Table 3.6; Fig. 3.S3b). On average across the three validation treatments NSE (~0.76) was very similar between the models. RZWQM2 performed better for CTRL1 and TRT2, however, DNDC performed better for CTRL2. Likewise, both models performed well for simulating monthly water flow to tiles with remarkably similar statistics. In all cases NSE was greater than 0.5. However, both models under-predicted water flow for TRT2 and over-predicted it for CTRL2. This could be attributed to variability in measurements since the standard error calculated from the 4 plot replicates was sometimes high, particularly in 2007 and 2008 when flow to drains was highest (Fig. 3.S5). Measurement variability was not accounted for in the statistics and the observations showed more overall water to tile drains in TRT2 (with cover crop) than in CTRL2 (without cover crop) which is unlikely. Both models predicted slightly more water loss to tile drains due to less transpiration when there was no cover crop. There was a simulated trade-off between evaporation and transpiration, but the cover crop was still predicted to reduce subsurface drainage volume which is consistent with some experimental studies (Strock et al., 2004; Qi and Helmers, 2010). A number of studies showed no effect of cover crop on subsurface water drainage volume (Drury et al., 2014b; Qi et al., 2011a; Qi et al., 2008; Kaspar et al., 2007). This could be due to the trade-off between reduced evaporation and increased transpiration when a cover crop was added in rotation and/or measurement variability masking a small influence.

Table 3.6 Statistical performance of DNDC and RZWQM2 for simulating water flow to tile drains from 2005-2009

	----- Calibration ----		---------------------------------- Validation	-----------------------------------				
	Treatment 1		Control 1		Treatment 2		Control 2	
	DNDC	RZWQM	DNDC	RZWQM	DNDC	RZWQM	DNDC	RZWQM
Annual (cm)								
NARE	1.6	6.0	-5.3	-1.4	-16.1	-13.3	17.5	24.5
r^2	0.98	0.93	0.85	0.93	0.96	0.97	0.88	0.80
NSE	0.97	0.92	0.83	0.90	0.78	0.83	0.73	0.47
Monthly (cm)								
r^2	0.73	0.67	0.70	0.76	0.68	0.66	0.68	0.69
NSE	0.73	0.67	0.71	0.76	0.65	0.65	0.62	0.60
Daily (cm)								
r^2	0.27	0.41	0.29	0.51	0.33	0.54	0.23	0.70
NSE	-0.32	0.35	0.08	0.50	0.24	0.50	-0.11	0.69

In a study by David et al. (2009) 6 models (SWAT, DayCent, EPIC, Drainmod-N II and two versions of DNDC, 82a and 82h) were compared for simulating aggregated water and nitrate flux to tile drains. It was found that all models except DNDC82h performed well in simulating monthly water flux (NSE>0.5), but the models which were designed to simulate tile drainage (SWAT, EPIC and Drainmod-N) demonstrated better performance (NSE>0.68). All of the models investigated included a cascade flow approach to simulating drainage. At this time the DNDC model versions tested included a Thornwaite approach, which sometimes greatly overestimates ET, thus it is not surprising that DNDC82h underestimated water loss to drains by 33%. In our current study, DNDC includes the Penman-Monteith approach with crop specific coefficients for ET (Dutta et al., 2016b) and the NSE for monthly flow to tiles was above 0.6 for all treatments. It is very important to simulate an appropriate level of ET, since it is usually the largest component of water loss.

The HERMES model, which includes cascade water flow, was previously used to simulate water and N loss to tile drains in a similar cropping system as used in our current study and it was found that once calibrated the model could simulate the lower N loss that occurred when cover crops were included in a corn-soybean cropping system with a reasonable degree of accuracy. The HERMES model was compared to RZWQM2, which was used to simulate the same cropping system in a previous study (Li et al., 2008). It was found that HERMES did not simulate the year to year variability in nitrate concentration nor the monthly drainage as well as did RZWQM2. Drainage was over-predicted in the September through December 2003-2005 period likely because HERMES did not include the reduced evaporation from residue cover. In our current study DNDC does include this impact and simulations of monthly water and N loss to drains were similar to RZWQM2. Both RZWQM2 and DNDC also include snow dynamics, which HERMES did not, and soil freeze-thaw processes. Late season drainage can be greatly overestimated without these processes which was the case for STICS in comparison to DNDC and DayCent in Guest et al. (2017a).

RZWQM2 performed substantially better than DNDC for simulating daily water flow (Table 3.6). The DNDC model tended to capture the start time of flow events but flow occurred too rapidly with over-prediction near the start of the event and under-prediction near the end. An example of this trend is shown in Fig. 3.5 for CTRL2 and the full comparison for 2007 and 2008, the years in which daily water flow was available (Qi et al., 2011b), is shown in Fig. 3.S6. This phenomenon can be expected from a cascade flow model which employs a bulk flux method for N and water movement and does not consider delays in drainage. It is important that the timing of these events are simulated correctly since soil water and oxygen content are critical drivers for denitrification and even short term erroneous predictions can greatly influence nitrous oxide emissions (Uzoma et al., 2015). A previous version of DNDC (DNDC87) included a recession curve to retain water in each layer, slowing drainage based on an empirical equation driven by clay content. This algorithm was developed by Li et al. (2006) and employed by Tonitto et al. (2007a, 2007b, 2010). We investigated re-enabling this routine in DNDC, on a test basis, and found that after parameterizing the recession curve for the calibration treatment the daily water flow was similar to RZWQM2 and statistics for the validation treatments were greatly improved to be as good as RZWQM2. However, soil water content was greatly over-predicted (NARE 21.8 %) resulting in exaggerated rates of denitrification and N_2O emissions were increased by 26%. Thus we do not recommend using this approach and it is not employed in the current U.S. DNDC release version.

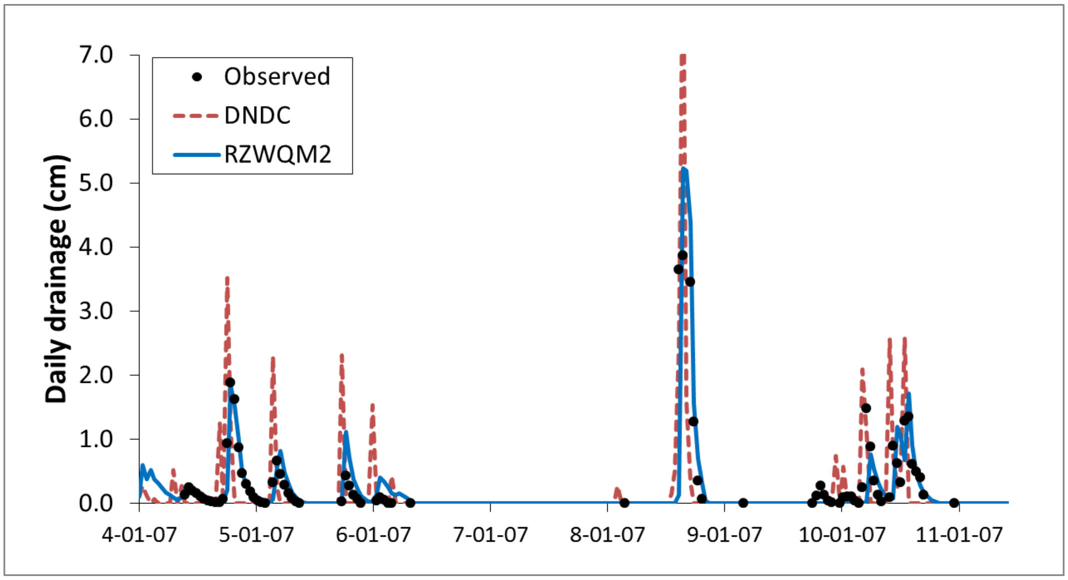

Figure 3.5 Observed and simulated daily water flow under soybean growth in 2007 for validation treatment CTRL2

3.3.3.2 Nitrogen loading to tile drains

Both models performed satisfactorily in estimating N loss to tiles on an annual basis (Table 3.7; Fig. 3.S3c), with similar average statistics across the validation treatments (NSE 0.72 and 0.65 for DNDC and RZWQM2, respectively). The models generally performed satisfactorily in simulating NO_3-N loss to tile drains on a monthly basis; however, DNDC performed a little better with acceptable statistics for CTRL2 (Table 3.7; Figure 3.6). David et al. (2009), when comparing the performance of 6 models, found that two different versions of DNDC predicted N loss to tiles within 10% but the monthly timing of N loss was relatively poorly simulated with NSE<0.4, which is considerably less than in our current study (Table 3.7). For all six models investigated David et al. (2009) indicated that inaccuracy in predicting the variation in monthly water flux resulted in inaccuracies in predicting N losses. Two of the three models which included tile drainage simulation performed better (SWAT and Drainmod-N II) with NSE>0.5.

In our study both DNDC and RZWQM2 agreed in estimating the magnitude of N loss to tile drains; however, similar to water flow to tile drains, both models underestimated loss in TRT2 and overestimated loss in CTRL2 (Table 3.7; Figure 3.S7). The observed and simulated cumulative water flow and N loss to tile drains on average across the 4 treatments was indeed very similar between the models and observations (Fig. 3.S8). The over and under predictions may be due to measurement variability amongst plots, especially when one considers that observations had greater average annual N loss in TRT2 (39.9 kg ha^{-1} y^{-1}) than in CTRL2 (33.7 kg ha^{-1} y^{-1}). This result seems unlikely considering that we generally expect less N loss to drains when a cover crop is included, which was the case for TRT1 (34.4 kg ha^{-1} y^{-1}) and CTRL1 (41.0 kg ha^{-1} y^{-1}). Both models consistently estimated less N loss to tile drains when a cover crop was included in rotation, which is a common finding in a number of experimental studies (Malone et al., 2017; Drury et al, 2014b; Li et al., 2008; Kaspar et al., 2007; Parkin et al., 2006; Strock et al., 2004; Logsdon et al., 2002). Qi et al. (2008, 2011c) did not find any difference in N loading when a cover crop was included in the study we simulated. This was likely because the winter during the 5 year experimental period was colder than usual leading to low winter rye biomass. In long term simulations over 40 years an 11% reduction of N loading was reported (Qi et al., 2011b).

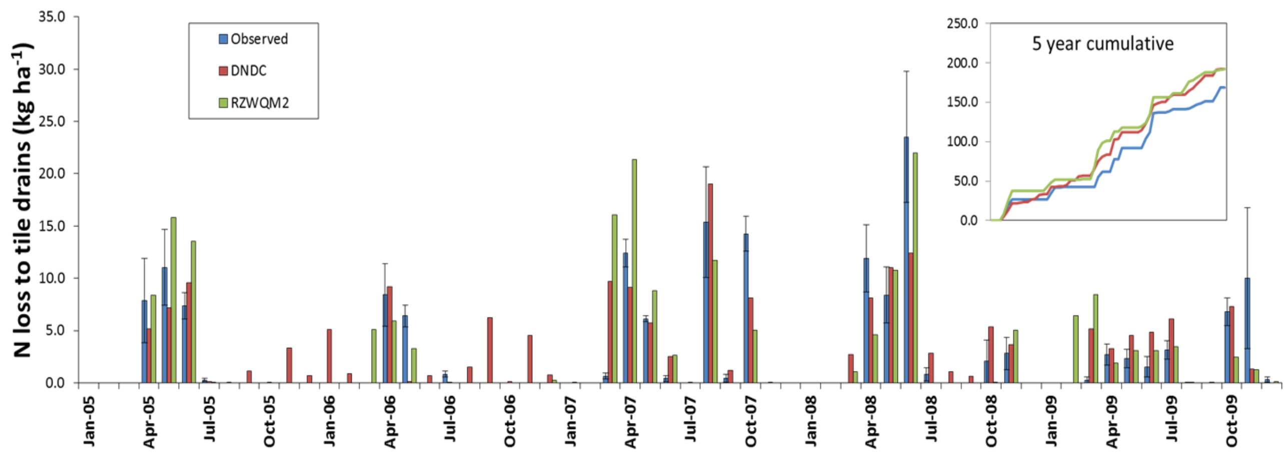

Figure 3.6 Observed and simulated monthly N loss to tile drains for the validation plot CTRL2 (2005-2009)

The observed rates of loss were generally high with an annual average loss of 37.3 kg NO_3-N ha^{-1} y^{-1} across all treatments. It may be expected that NO_3-N leaching is high in a well-drained soil with subsurface drainage but runoff of phosphorous, sediment, NH_4-N and NO_3-N is generally low (Lawlor et al., 2008). In this study there were no observations available for runoff but both models predicted minimal NO_3-N runoff (<1 kg N ha^{-1} y^{-1}) for all years and treatments which was expected for this site.

Table 3.7 Statistical performance of DNDC and RZWQM2 for simulating nitrogen loss to tile drains from 2005-2009

	----- Calibration ----		---------------------------------- Validation	-----------------------------------				
	Treatment 1		Control 1		Treatment 2		Control 2	
	DNDC	RZWQ2	DNDC	RZWQ2	DNDC	RZWQ2	DNDC	RZWQ2
Annual (kg ha^{-1})								
NARE	7.4	0.2	-3.0	-1.4	-10.7	-17.8	14.1	13.7
r^2	0.89	0.93	0.91	0.70	0.65	0.98	0.87	0.78
NSE	0.85	0.92	0.86	0.68	0.56	0.73	0.73	0.53
Monthly (kg ha^{-1})								
r^2	0.54	0.68	0.65	0.68	0.63	0.52	0.59	0.56
NSE	0.53	0.67	0.65	0.67	0.59	0.51	0.58	0.44

3.4 Conclusions

It is important to continue to scrutinize and compare agriculture models against high quality datasets to identify differences in model structure that result in improved performance. Sometimes during model development there are options to include more complex processes and model structure, however, a developer may purposefully keep the inputs and complexity manageable in order to minimize input requirements and reduce the level of required modeler expertise. In this study we compare the performance of two widely used process-based models for simulating crop growth and soil water dynamics and NO_3-N loss to tile drains. The conceptual design of each of these models was focused on different objectives. The DNDC model was mostly developed and employed for simulating GHG emissions and soil carbon change whereas RZWQM2 focused primarily on crop growth and water quality.

It was informative to discover that a simple cascade water sub-model (DNDC) performed adequately in comparison to measurements and similarly with respect to RZWQM2 across a wide range of metrics including crop yield, biomass, N uptake of winter rye, annual and monthly water flow and NO_3-N loss to tile drains. The Penman-Monteith method for estimating ET in DNDC, recently improved by Dutta et al. (2016b), was a strong factor in estimating the appropriate water balance, particularly since ET was estimated to be a large percent of the water budget. It was interesting to find that bulk gravity drainage regulated by cascade water flow through a homogeneous soil profile was effective in simulating water flow on an annual and monthly basis, but not on a daily basis. If this scale of resolution is deemed appropriate for the study objective, then no further detail in hydrologic processes may be needed.

Estimates from DNDC did reveal shortcomings in simulating soil water storage, soil water contents down the profile and daily water flow events whereas RZWQM2 generally performed adequately for these metrics. Fine scale temporal simulation of water and N dynamics can greatly impact soil water and nutrient levels, thereby influencing several biogeochemical processes such as decomposition, denitrification, nitrification and methanogenisis. These processes are largely dependent on soil water content. Since DNDC is primarily used to simulate GHG emissions we recommend that developments be carried out for DNDC to further improve its hydrological processes. Such changes may include a deeper and heterogeneous soil profile, inclusion of root distribution functions, inclusion of improved water flow, a fluctuating water table, and/or a mechanistic drainage sub-model. A mechanistic tile drainage sub-model could also enable the simulation of the impacts of drainage depth and spacing, controlled drainage and irrigation on nutrient cycling and GHG emissions, which would greatly increase the usefulness of an already widely used model. Considerations should, however, be taken when contemplating model developments. More complex processes can increase model input requirements, inputs which may not be available, especially in regional large scale studies. Pedo-transfer functions are sometimes used to estimating soil-water inputs for models, but they also come with a degree of uncertainty. Most of the suggested additions for DNDC likely would not greatly increase model input requirements or simulation time, however, it remains questionable whether or not to include a computationally intensive water flow approach (i.e. the Richards Equation).

3.5 Supplementary Tables and Figures

Table 3.S1 Measured soil physical and hydraulic properties (adapted from Qi et al., 2011b)

Depth (cm)	Sand (%)	Clay (%)	BD (g cm^{-3})	SOM (%)	K_{sat} (cm h^{-1})	Porosity	Θ_{10} (cm^3 cm^{-3})	Θ_{33} (cm^3 cm^{-3})	Θ_{1500} (cm^3 cm^{-3})
0-10	0.32	0.32	1.37	4.3	4.8	0.482	0.383	0.376	0.189
10-20	0.32	0.32	1.38	3.8	3.3	0.476	0.384	0.376	0.230
20-30	0.33	0.14	1.39	3.3	5.1	0.473	0.384	0.376	0.201
30-40	0.4	0.30	1.39	1.3	4.1	0.474	0.384	0.399	0.212
40-60	0.46	0.24	1.39	1.3	4.1	0.474	0.408	0.368	0.218
60-90	0.44	0.20	1.45	0.6	2.6	0.450	0.38	0.368	0.204
90-120	0.44	0.20	1.46	0.5	2.6	0.450	0.312	0.299	0.184
120-200	0.44	0.20	1.46	0.5	2.6	0.450	0.31	0.299	0.168
200-300	0.44	0.20	1.50	0.5	2.6	0.450	0.31	0.299	0.168
300-390	0.44	0.20	1.50	0.5	0.01	0.450	0.31	0.299	0.168

BD = bulk density; SOM = soil organic matter; K_{sat} = saturated hydraulic conductivity; θ_{10}, θ_{33}, θ_{1500} = soil water content at pressure 10, 33 and 1500 Kpa, respectively

Table 3.S2 Calibrated crop parameters used in RZWQM2 for corn, soybean and winter rye

Crop	Parameter	Parameter description	Value
Corn[a]	G2	Maximum possible number of kernals per plant	722
	G3	Kernel filling rate during linear grain filling stage under optimum conditions (mg d^{-1})	6.55
	PHINT	Phylochron interval between successive leaf tip appearance	46
Soybean[b]	LFMAX	Max leaf photosynthesis rate (μmol CO_2 m^{-2} s^{-1})	0.8
Winter rye[c]	PEG	Germination phase duration (°C d cm cm^{-1})	75
	PECM	Emergence phase duration (°C d cm cm^{-1})	25
	P1V	Relative amount that development is slowed for each day of unfulfilled vernalization, assuming 50 d is sufficient	5
	P1D	Relative amount that development is slowed when plants are grown in photoperiod 1 hour shorter than optimim (d)	12
	PARUV	Conversion rate for photosynthetically active radiation to dry matter before the end of leaf growth (g MJ^{-1})	3.3
	LAVS	Area of standard vegetative stage leaf (cm^2)	15
	LARS	Area of standard reproductive phase leaf (cm^2)	25
	LARWS	Lamina area to weight ratio of standard first leaf (cm^2 g^{-1})	300
	LAWR2	Lamina area to weight ratio, phase 2 (cm^2 g^{-1})	280
	P5	Relative grain filling duration based on thermal time (d)	400
	PHINT	Phylochron interval between successive leaf appearance (PD)	100

[a] Cultivar IB1 068 Dekalb 521
[b] Cultivar 990002 M Group 2
[c] Cultivar 990003 Winter-US

Table 3.S3 Statistical performance of DNDC and RZWQM2 for simulating soil water storage (cm^3 cm^{-3}) from 2005-2009

	----- Calibration ----		-------------------------------- Validation				---------------------------------	
	Treatment 1		Control 1		Treatment 2		Control 2	
	DNDC	RZWQ2	DNDC	RZWQ2	DNDC	RZWQ2	DNDC	RZWQ2
NARE	1.9	1.1	4.6	4.3	0.81	1.88	2.8	4.5
NRMSE	9.2	4.7	11.5	6.0	10.5	4.7	10.7	6.4
r^2	0.51	0.61	0.51	0.63	0.56	0.66	0.59	0.55
RSR	1.43	0.73	2.34	1.23	2.15	0.95	1.67	1.02
NSE	-1.05	0.46	-4.52	-0.52	-3.61	0.08	-1.18	-0.03

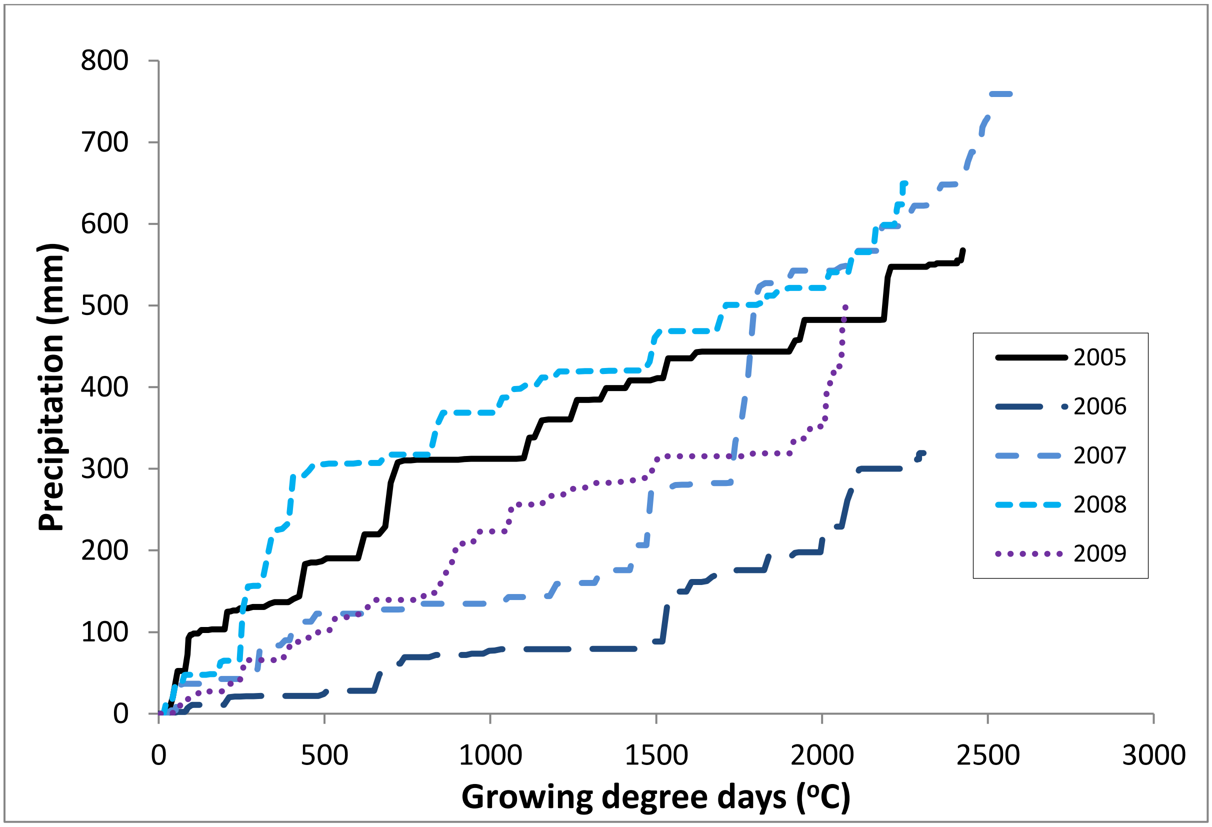

Figure 3.S1 Cumulative precipitation vs. cumulative GDD during the growing seasons from 2005 to 2009.

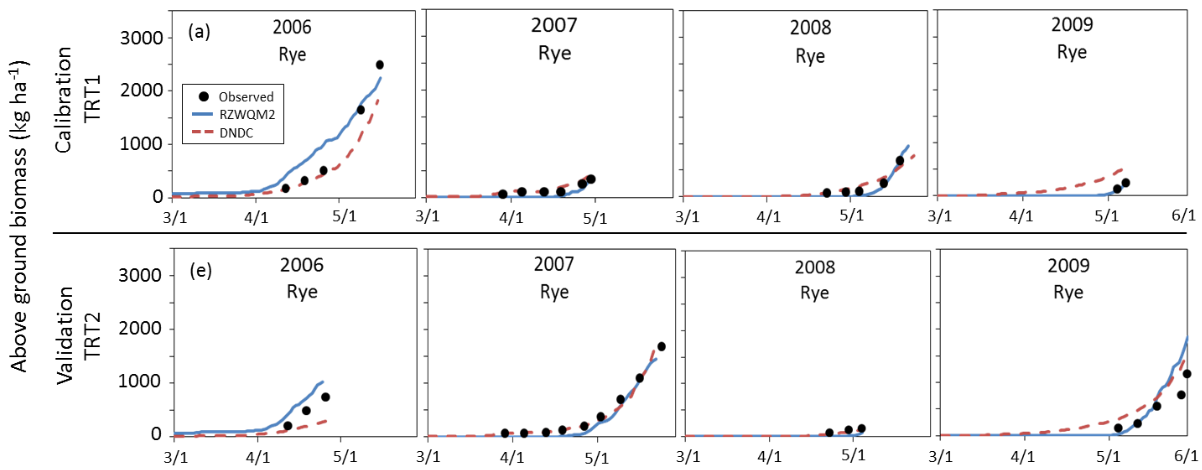

Figure 3.S2 Measured and modelled rye dry biomass from 2006 to 2009 for a) calibration plot TRT1 (a-d) and validation plot TRT2 (e-h).

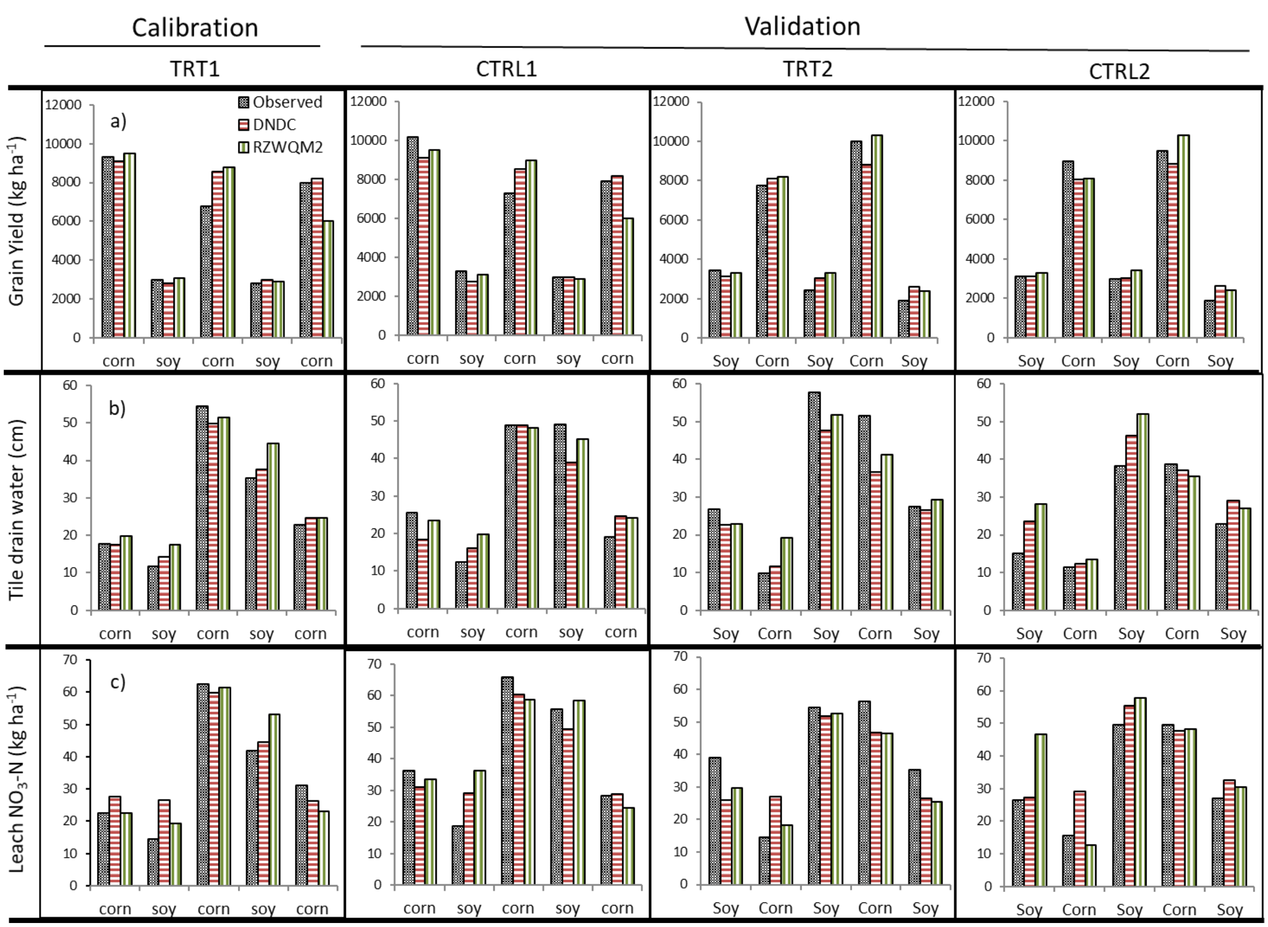

Figure 3.S3 Annual a) corn and soybean crop yield, b) water flow to tile drains and c) N loss to tile drains from 2005 to 2009

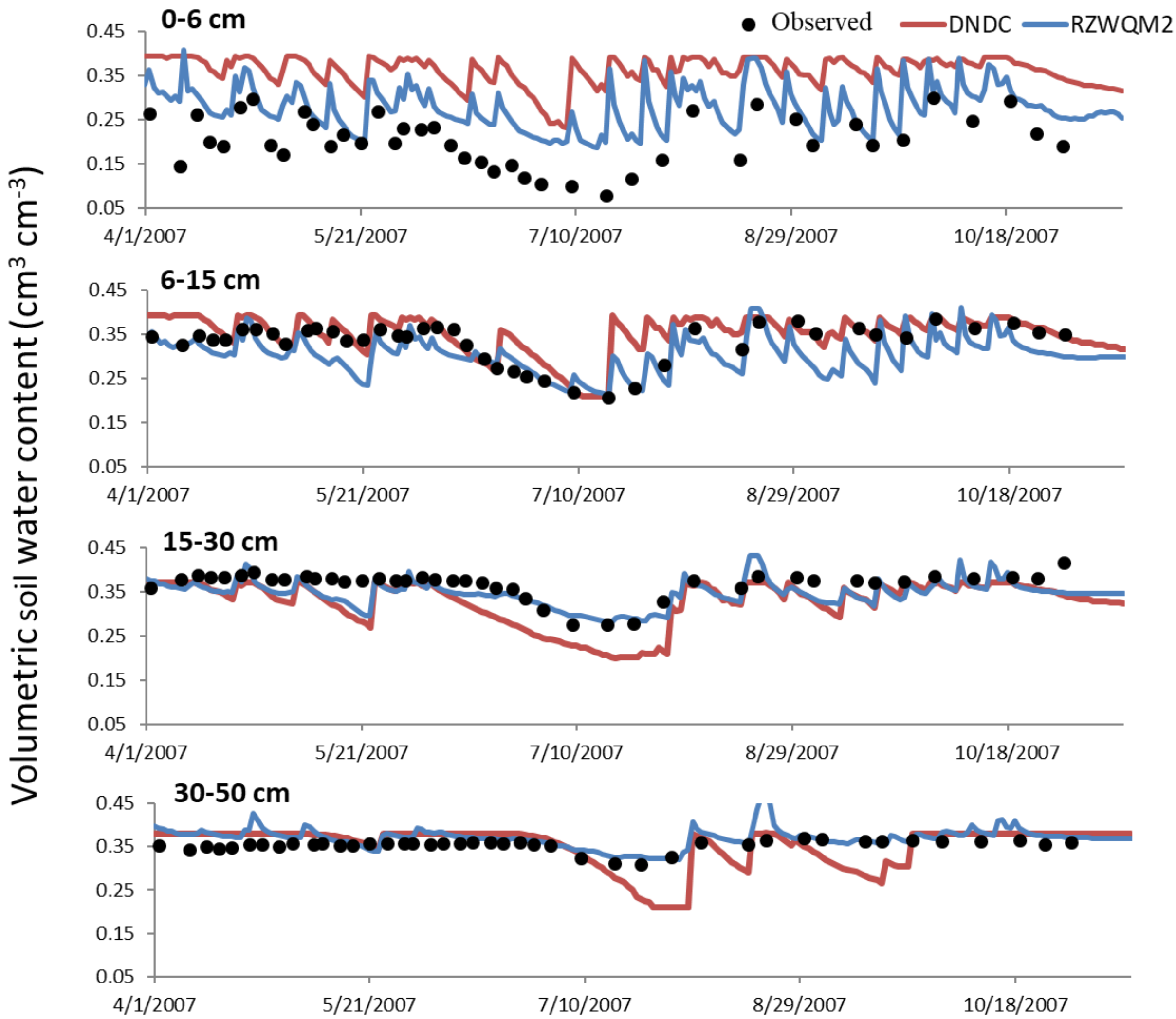

Figure 3.S4 Example of soil water content by profile layer, validation TRT2 in 2007

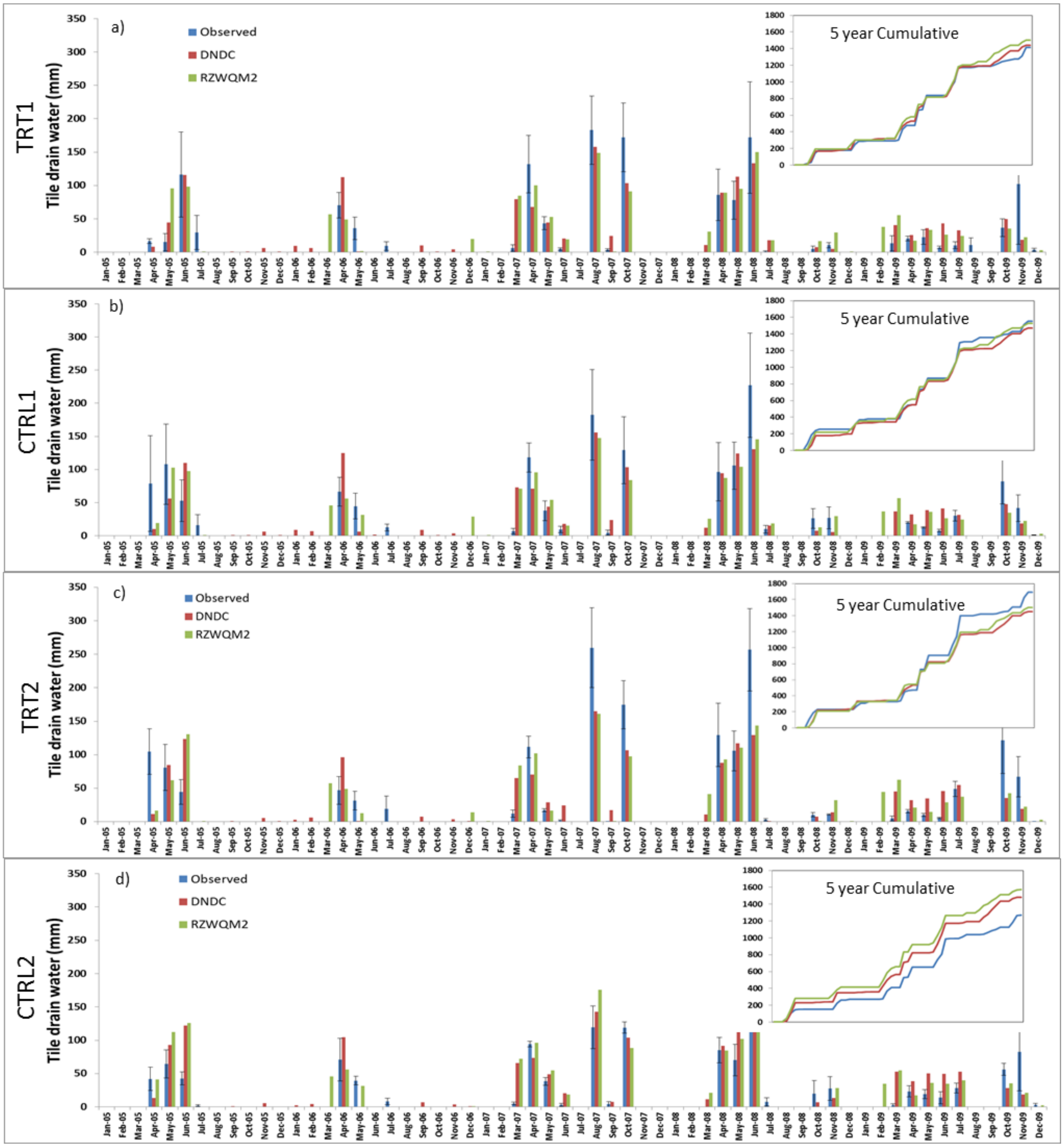

Figure 3.S5 Observed and simulated monthly water flow to tile drains for the calibration plot TRT1 (a), and the validation plots b) CTRL1, c) TRT2, and d) CTRL2 (2005-2009).

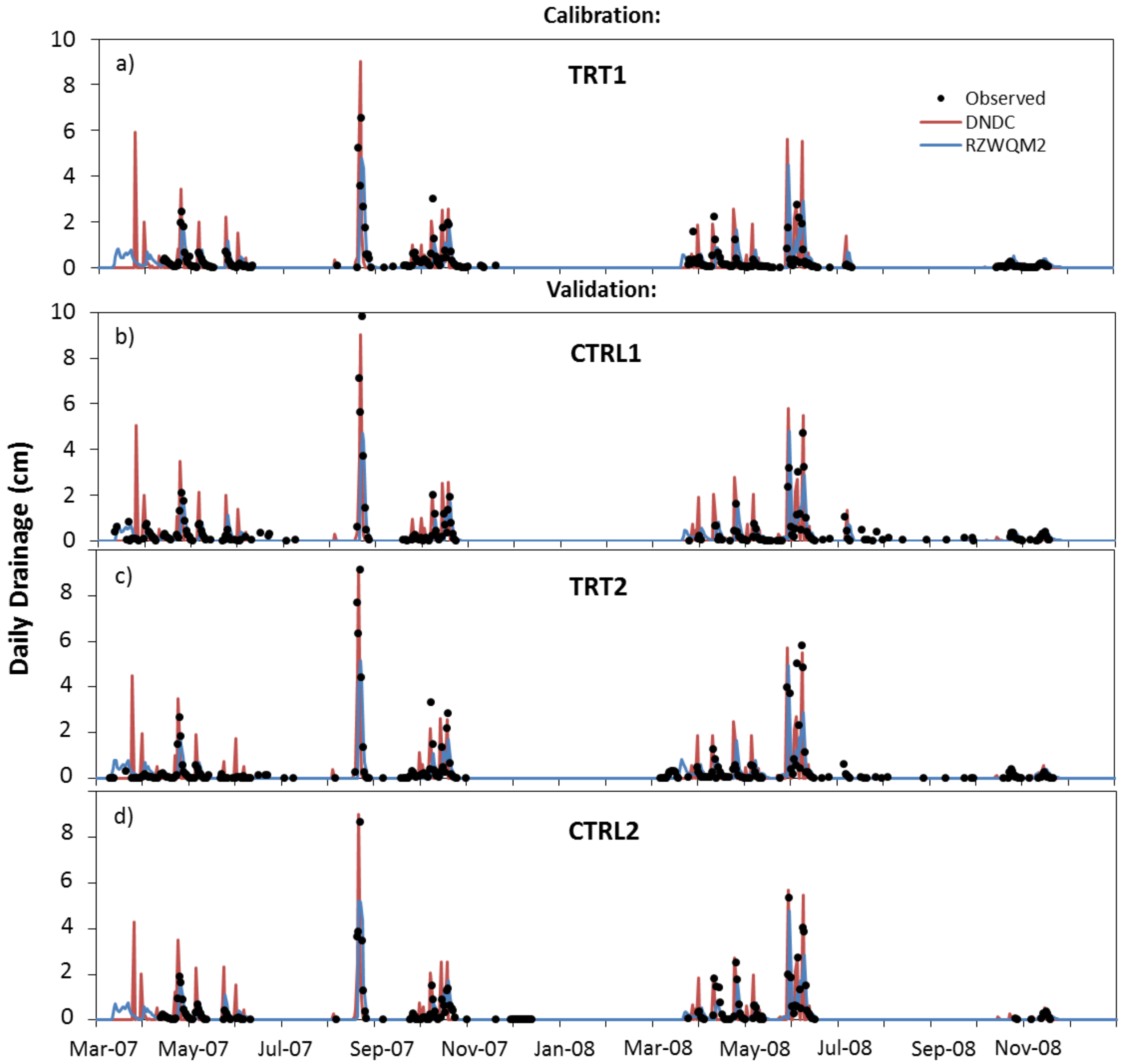

Figure 3.S6 Observed and simulated daily water flow to tile drains for the calibration plot TRT1 (a), and the validation plots b) CTRL1, c) TRT2, and d) CTRL2 (2007-2008).

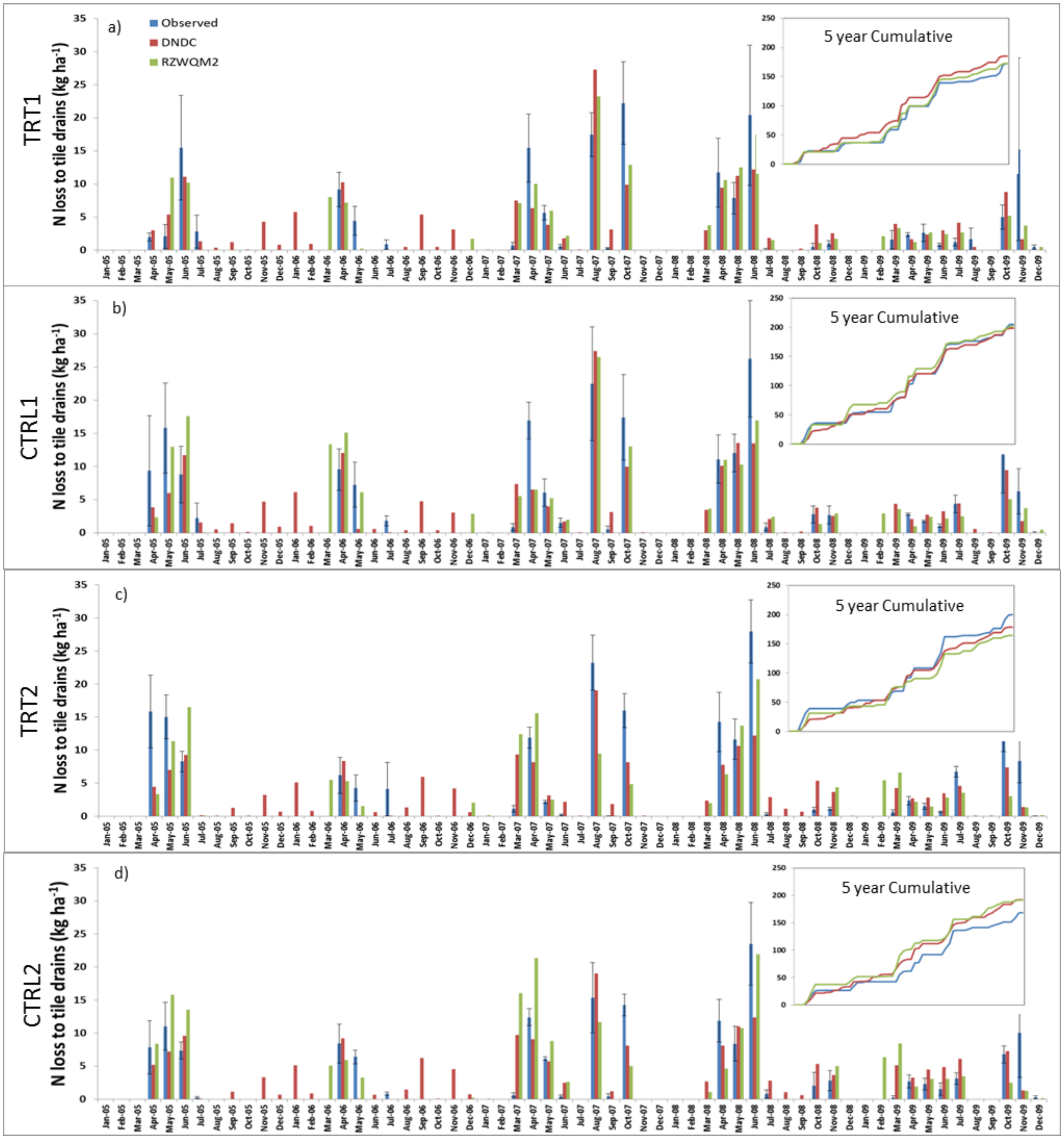

Figure 3.S7 Observed and simulated monthly N loss to tile drains for the calibration plot TRT1 (a), and the validation plots b) CTRL1, c) TRT2, and d) CTRL2 (2005-2009).

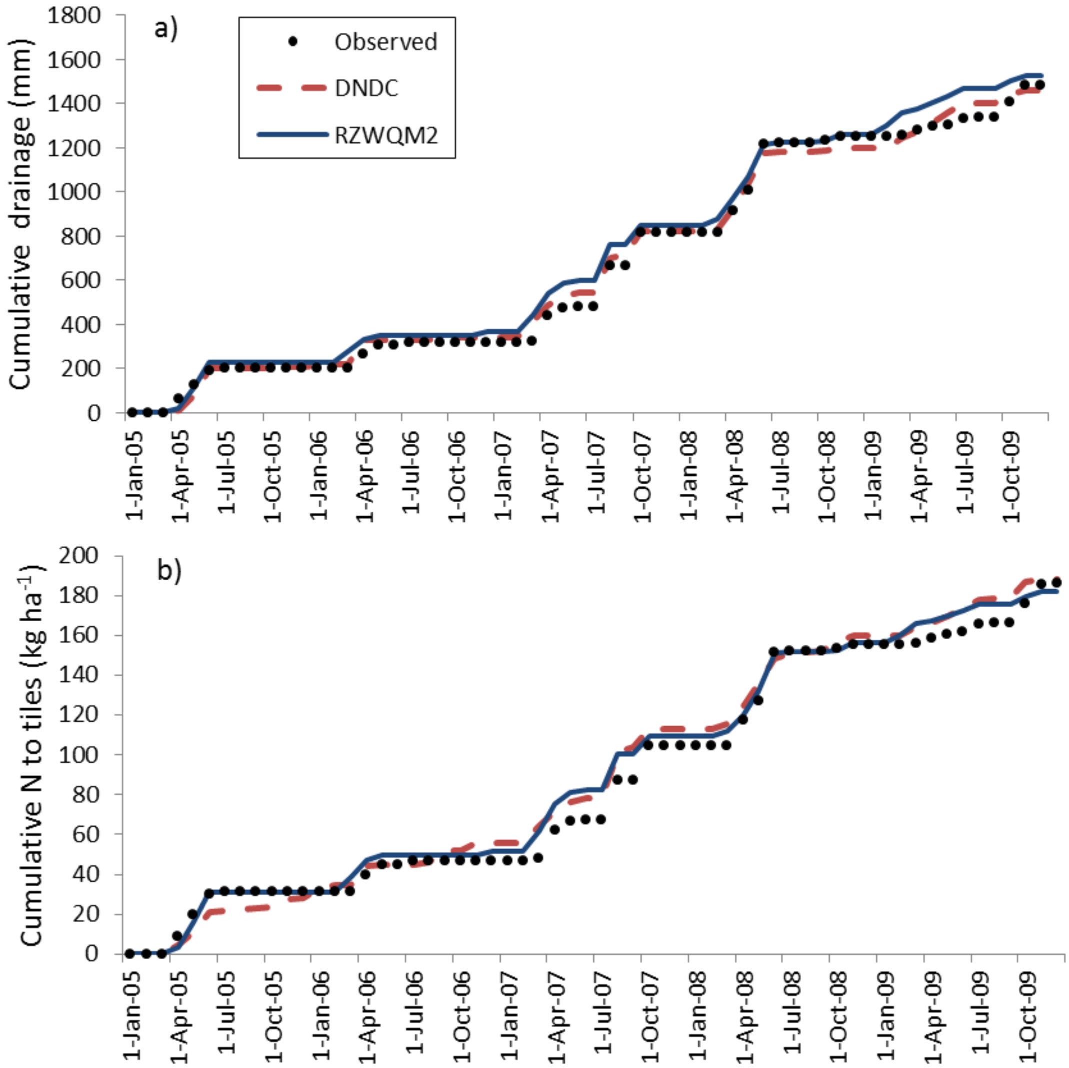

Figure 3.S8 Observed and simulated cumulative a) water flow and b) N loss to tile drains as an average across the 4 treatments (2005-2009).

Connecting text to Chapter 4

The first step in understanding which hydrologic processes in DNDC required improvements was largely accomplished in Chapter 3 whereby the model outcomes were compared to detailed observed data and to results from RZWQM2. Additionally, in Chapter 2, numerous recent studies are documented which acknowledge flaws in the simulation of soil water and the adverse impacts this can have on the simulation of biogeochemical processes in DNDC. In Chapter 4 restructuring and improvement of the hydrological framework in DNDC was undertaken to increase the simulation depth and include a heterogeneous soil profile, fluctuating water table, root density functions, and tile drainage sub-model. In doing so, alternative hydrologic processes were investigated with considerations for not only accuracy, but also for the level of computational, input data and expertise required to employ the model. The DNDC model was again compared to RZWQM2 using the same observed data as in Chapter 3, but also, additional site data was included with observed impacts of controlled drainage and sub-irrigation on water and N losses.

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Chapter 4

Development of the DNDC model to improve soil hydrology and incorporate mechanistic tile drainage: A comparative analysis with RZWQM2

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Abstract

The Denitrification Decomposition model (DNDC) has known limitations for simulating soil hydrology which can strongly influence biogeochemical processes. For this study, DNDC's soil hydrological framework was enhanced by including a new sub-model for mechanistic tile drainage, improved water flux, root growth dynamics, and a deeper and heterogeneous soil profile. Comparisons were then conducted against the Root Zone Water Quality model (RZWQM2), using measurements of soil water storage, runoff and drainage in eastern Canada and the US Midwest. Simulation of soil water storage (DNDC $0.81 \leq d \leq 0.90$; RZWQM2 $0.76 \leq d \leq 0.84$), daily water flow (DNDC $0.76 \leq d \leq 0.88$; RZWQM2 $0.77 \leq d \leq 0.90$) and nitrogen loading to tile drains was greatly improved post-development, where d is the Wilmott index of agreement. DNDC was able to capture the observed differences in water and N losses between conventional drainage and controlled drainage management with sub-irrigation. The enhancements to DNDC's hydrological framework should increase its performance for simulating several biogeochemical processes.

4.1 Introduction

Efficient management of water and nutrients in agricultural systems is essential to further improve profitability for producers and to reduce greenhouse gases (GHG), losses of excess nitrogen (N), phosphorus and ammonia, which can contribute to global warming, eutrophication of water bodies and increases in atmospheric fine particulate matter. When considering the long-term sustainability of agriculture, it is of great importance to examine the interrelationships and trade-offs between crop productivity and all environmental outcomes.

There are numerous field and laboratory studies worldwide which focus on mitigating losses of nutrients, reducing GHG emissions and sequestering soil carbon in agricultural systems. However, due to extreme spatial and temporal variability in soils and climate, tools are required for extrapolating the knowledge gained from these studies over space and time. Because process based models, such as DayCent (del Grosso et al., 2001), the DeNitrification DeComposition model (DNDC; Li et al., 2012), the Root Zone Water Quality Model (RZWQM2; Ma et al., 2012) and APSIM (Thorburn et al., 2018), can dynamically simulate many of the interdependent process while maintaining a strict mass balance of nutrients and water, they are valuable for predicting N losses in the environment and assisting in the selection of best management practices (BMPs) (De Jong et al., 2009). While they offer valuable opportunities for expanding the scope of existing assessments, such models still have recognized knowledge gaps and thus require new targeted measurements for the development of improved mechanisms to ensure that the iterative process for model development continues. For instance, model structure is often limited by the oversimplified representation of soil and hydrological processes. In a review of nine GHG models, Brilli et al. (2017) found that 46% of the deficiencies in models were due to issues with the simulation of pedo-climatic conditions including soil-water simulation. In the same review DNDC was found to be the only model which simulated all C&N related GHG emissions considered. The DNDC model is the most prominent process-based model used for simulating GHG emissions worldwide, however, it has known issues in simulating soil hydrology (Smith et al., 2019c; He et al., 2019a, 2018; Brill et al., 2017; Congreves et al., 2016b; Dutta et al., 2016b; Cui et al., 2014; Abdalla et al., 2011; Deng et al., 2011). These deficiencies impact the performance of the model for simulating C&N cycling and the timing of N_2O emissions (He et al., 2018a; Uzoma et al., 2015; Smith et al., 2008). As a result, it has been suggested in many of these studies that DNDC development should be focused on improving the simulation of soil hydrology.

Several iterations of the DNDC model have been developed for different regions globally including New Zealand DNDC (Saggar et al., 2007), Landscape DNDC (Hass et al., 2013), China DNDC (Li et al., 2017) and Canada DNDC (Smith et al., 2013). Each one of these models can still be applied globally but they were developed to include additional processes and management options relevant to the locations where they were developed. In the case of the Canada DNDC model (DNDC.vCAN), it was designed to better simulate soil-plant–climate interactions in cool weather climate and has recently been improved for simulating evapotranspiration (Dutta et al., 2016b), ammonia volatilization (Dutta et al., 2016a; Congreves et al., 2016b), impacts of snow cover and residue on soil temperature (Dutta et al., 2018), and improved growth of cool weather crops (He et al., 2019a; Grant et al., 2016; Kroebel et al., 2011). Further, model developments from Canada DNDC were integrated back into the primary U.S. release version (Smith et al., 2019c). However, as with any model, there remain shortcomings in the current model framework. Grant et al. (2016) identified that mineralization rates were too low in DNDC, sometimes resulting in excessive crop N stress. This can largely be attributed to the limitation that DNDC only simulates soil C&N processes over a 50 cm soil horizon. Also, in a detailed assessment of water processes in Canada DNDC, Smith et al. (2019c) found that DNDC predicted crop biomass and monthly water and N flow to tile drains well but did poorly in predicting soil water content and daily tile flow events. In the same study, another model, RZWQM2, using more computational intensive hydrological processes, predicted good results but RZWQM2 requires more expertise to employ, greater simulation time, and is not well validated for simulating some biogeochemical processes. Since soil biogeochemical processes including chemical equilibria, nitrification, denitrification and fermentation are highly dependent on soil water content Smith et al. (2019c) recommended the inclusion of a heterogeneous profile that exceeds crop rooting depths, root density functions, improved water flow and mechanistic tile drainage.

There is considerable complexity in developing improved soil structure, hydrology and tile drainage in DNDCv.CAN, while ensuring that the reliant biogeochemical mechanisms still function appropriately, but research has indicated that these improvements are critical and long overdue towards the evolution of the model. An accurate estimate of soil hydrology is important for predicting the timing of N_2O emissions and N leaching events. Therefore, the objectives of this study were i) to improve DNDC for simulating soil hydrology, including the addition of a heterogeneous and deeper soil profile, root density functions, and improved water flow, ii) to incorporate a mechanistic tile drainage sub-model and include the ability to simulate a fluctuating water table, controlled drainage and sub-irrigation, and iii) to compare the performance of DNDC to the computationally intensive RZWQM2 using detailed datasets of runoff and drainage in eastern Canada and the US Midwest. It was deemed important that model developments be implemented at the minimum level of complexity and computation time necessary for improving accuracy, while keeping the user expertise at a manageable level.

4.2 Materials and methods

4.2.1 Description of Experimental sites

4.2.1.1 Gilmore City, Iowa, USA experimental site

A five-year field experiment was established in the fall of 2004 and lasted until the end of 2009 at the Agicultural Drainage and Water Quality – Research and Demonstration Site close to Gilmore City in north central Iowa, USA. The site soils are predominantly characterized as Nicollet (fine-loamy, mixed, superactive Aquic Hapludoll), Webster (fine-loamy, mesic Typic Endoaquolls), Canisteo (fine-loamy, mesic Typic Endoaquolls), and Okoboji (Fine, smectitic, mesic Cumulic Vertic Endoaquolls). General site characteristic are shown in Table 4.1 and detailed soils data by horizon are presented in Table 4.S1. Four land cover treatments were initiated with the first two consisting of alternating phases of winter rye cover crop prior to maize or prior to soybean (first phase of the rotation TileDrain-CoverCrop-MaizeSoybean [TD-CC-MS] and second phase of the rotation TileDrain-CoverCrop-SoybeanMaize [TD-CC-SM]). The next two treatments were alternating phases of maize and soybean with no cover crop (first phase of rotation TileDrain-NoCoverCrop-MaizeSoybean [TD-NCC-MS] and second phase of rotation TileDrain-NoCoverCrop-SoybeanMaize [TD-NCC-SM]) (Table 4.2). Aqueous ammonium nitrogen was applied to maize at a rate of 140 kg N ha^{-1} in the spring near emergence time. The site includes a large compliment of measurements including water content across 4 depths, crop yields, biomass and daily measurement of water flow and N concentration to tile drains. See Qi et al. (2011a, b) for a more detailed description of soil, management and experimental setup.

Table 4.1 Site characteristics at Gilmore City and Woodslee research plots

Location and data collection period	Soil classification*	Average annual temp. (ºC)	Average annual precip. (mm)	Average growing season precip. (mm)	Soil characteristics			
					Soil surface texture (%)	Soil Organic Carbon (g kg^{-1})	pH	Bulk density (g cm^{-3})
Woodslee, Ontario, Canada 42°13'N, 82°44'W (1999-2005)	Poorly drained, fine, loamy, mixed, mesic, Typic Argiaquoll	9.8	816	491	28 sand 35 silt 37 clay	25.0	7.0	1.42
Gilmore City, Iowa, United States 42°42'N 104°00'W (2005-2009)	Nicollet (fine-loamy, mixed, superactive, mesic Aquic Hapludoll)	8.7	824	578	32 sand 34 silt 32 clay	23.2	7.1	1.37

* Other soil series are also present at the Gilmore City site.

Table 4.2 Cropping systems and agronomic practices at the Gilmore City site, Iowa from 2005 to 2009 (adapted from Smith et al., 2019c)

	2005	**2006**	**2007**	**2008**	**2009**
Treatment					
TD-CC-MS, Calibration	rye-maize	rye-soy.	rye-maize	rye-soy.	rye-maize
TD-NCC-MS, Validation	maize	soybean	maize	Soybean	maize
TD-CC-SM, Validation	rye-soy.	rye-maize	rye-soy.	rye-maize	rye-soy.
TD-NCC-SM, Validation	soybean	maize	soybean	maize	soybean
Management activity					
Termination of rye prior to maize	April 30	April 24	April 30	May 6	May 8
Cultivation(a) and maize planting	May 10	May 4	May 14	May 15	May 19
Cultivation(a) and soybean planting(b)	May 18	May 10	May 17	May 23	May 20
Termination of rye	May 20	May 16	May 23	May 26	May 31
Maize fertilizer (@140 kg N ha^{-1})	May 25	May 18	June 5	June 4	June 30
Maize and soybean harvest	Oct. 10	Oct. 7	Oct. 22	Oct. 20	Nov. 3
Chisel plow (NCC rotations)	Oct. 10	Oct. 10	Oct. 24	Oct. 20	no-till (wet)
Disk and cultivation (CC rotations)	Oct. 10	Oct. 10	Oct. 24	Oct. 20	no-till (wet)
Plant rye	Oct. 11	Oct. 12	Oct. 25	Oct. 21	Nov. 20

a) Only TD-NCC-MS and TD-NCC-SM were cultivated
b) DNDC handles intercropping but not RZQWM2, thus for RTWQM2 soybean was planted after rye termination

4.2.1.2 Woodslee, Ontario, Canada experimental site

A study was conducted at the Honorable Eugene F. Whalen Experimental Farm, Woodslee, Ontario Canada (42°13'N, 82°44'W) to monitor surface runoff and tile drainage (Drury et al., 2014b). The Brookston clay-loam soil at the site is classified as an Orthic Humic Gleysol (Canadian Classification system) or a poorly drained, fine, loamy, mixed, mesic, Typic Argiaquoll in the USDA system (Table 4.1, 4.S1). The study was of 5 years duration starting in late 1999 and ending in early 2005 (Table 4.3). Treatments included a maize-soybean rotation and unrestricted tile drainage with (TD-CC-MS) and without (TD-NCC-MS) a winter wheat cover crop and also controlled drainage and sub-irrigation with (CDS-CC-MS) and without (CDS-NCC-MS) a cover crop. This data helped to facilitate testing the new controlled drainage/sub-irrigation feature in DNDC. Both a starter (18-46-0) and sidedress application of UAN (150 kg N ha^{-1}) was applied to maize for a combined nitrogen rate of 175 kg N ha^{-1}. Maize grain was harvested in early November and tillage generally consisted of fall disking except when excessive residue required a more substantial cultivated heavy plough. Two flow meters were used in each plot to measure cumulate surface runoff and drainage flow. Samples of surface water and runoff were collected using an autosampler every 500 to 3000 L of flow and analysed for NO_3^- concentration. In the plots with controlled drainage and sub-irrigation treatments, controlled drainage was initiated at 0.3 m below the soil surface in the spring or early summer of each year and was maintained during the entire growing season. Sub-irrigation was applied by pumping water from an adjacent irrigation pond into control structures which flowed up the tile drains. This was applied in the dryer years from from 9 July to 17 August in 2001 (148 mm for CDS-NCC-MS and 106 mm for CDS-CC-MS) and from 16 July to 22 August in 2002 (85 mm for CDS-NCC-MS and 106 mm for CDS-CC-MS).

From June to July 2001 intact soil cores were collected for determination of bulk density, saturated hydraulic conductivity and soil water retention at 9 matric potentials. See Drury et al. (2014b) for a more detailed description of soil, management and experimental setup.

Table 4.3 Cropping systems and agronomic practices at the Woodslee site, from 2000 to 2005

	2000	2001	2002	2003	2004	2005
Treatment						
TD-CC, Calibration	ww-maize	ww-soy.	ww-maize	ww-soy.	ww-maize	ww-soy.
TD-NCC, Validation	maize	soybean	maize	soybean	maize	soybean
CDS-CC, Validation	ww-maize	ww-soy.	ww-maize	ww-soy.	ww-maize	ww-soy.
CDS-NCC, Validation	maize	soybean	maize	soybean	maize	soybean
Management activity						
Termination of ww*	May 8	May23	May 21	May 27	June 3	May 19
Plant soybeans		June 8		June 17		May 31
Plant maize and starter (25 kg N ha^{-1})	May 17		May 22		June 4	
Sidedress (UAN 150 kg N ha^{-1})	June 22		June 18		June 22	
Soybean harvest		Nov 6		Oct 6		Oct 26
Maize harvest	Nov 8		Nov 4		Nov 10	
Fall disking	Nov 8	Nov 6	Nov 6	Nov 6	Nov 22	
Plant winter wheat	Nov 8	Nov 7	Nov 7	Nov 7	Nov 23	

ww – winter wheat
* Roundup (1.4 kg ha^{-1} a.i.) was used to terminate ww in 2000, 2003, and 2004 whereas Vantage (1.4 kg ha^{-1} a.i.) was used in 2001 and 2002. All plots were sprayed.

4.2.2 Model description

4.2.2.1 DNDC model

The DNDC model was developed originally to simulate N_2O emissions (Li et al., 1992) and gained popularity due to its detailed biochemical equations describing nitrification and denitrification processes. It was later expanded to simulate soil C&N cycling, water and N movement (Li et al., 2006) and full farm nutrient cycling (Li et al., 2012) and now contains sub-models for simulating crop biomass, decomposition, nitrification denitrification, fermentation and ammonia volatilization. The model simulates a very wide array of agricultural management and crop types, the input requirements are reasonable and it can be applied with relative ease. As a result, DNDC has been used extensively worldwide (Ehrhardt et al., 2018; Brilli et al., 2017; Zhang and Niu, 2016; Gilhespy et al., 2014; Giltrap et al., 2010). Many users have, however, reported that the model had issues in simulating soil water content (Smith et al., 2019c; He et al., 2018a; Brilli et al, 2017; Congreves et al., 2016b; Dutta et al., 2016b; Uzoma et al., 2015; Smith et al., 2008; Cui et al., 2014; Abdalla et al., 2011; Deng et al., 2011) which is correlated with soil oxygen content, a driver for the growth and death of nitrifier and denitrifier bacteria in DNDC. Since soil water content impacts the type and rate of microbial reactions in DNDC it can greatly impact N_2O emissions. Furthermore, since DNDC only simulates soil C&N cycling to a 50 cm depth, processes such as nitrification, denitrification, nitrate leaching, fermentation, ammonium fixation, and mineralization may be represented inaccurately to account for the limited depth of simulation.

DNDC employs a simple layered cascade approach for simulating bulk water flux and N transport down the soil profile. Water drains to field capacity in each layer (~2cm thickness) at the rate of K_{SAT} (Fig. 4.1). Both water flow and C&N cycling are simulated to 50 cm depth through a homogeneous soil profile. A deep water pool, with a water holding capacity based its bulk density, is situated below the 50 cm soil profile to provide water for crop transpiration (50 cm soil profile + 50 cm deep water pool=100 cm total water pool). The model rooting depth is fixed with transpiration being drawn equally across all soil layers, followed by extraction from the deep water pool when plants are under water stress. To improve the simulation of water and N loss to tiles Li et al. (2006) incorporated a simple “recession curve” to delay drainage by soil layer but this is not active in the current U.S. DNDC release version. Smith et al. (2019c) tested this approach and although the simulated drainage was improved soil water content was then overestimated by 22% and N_2O emissions increased by 26%.

Since 2011 a Canadian version of DNDC (now referred to as DNDCv.CAN) has been under development to improve the simulation of agricultural management and crop cultivars in cool weather climate. The model version can still be employed worldwide since the default crop growth sub-model is available as an option. In 2017, developments from Canada DNDC were merged into the U.S. DNDC release version and thus developments from both model versions became available (Smith et al., 2019c). In addition to improving the model for simulating crop growth (Kroebel et al., 2011; Grant et al., 2016; He et al., 2019a) the simulation of several processes were also improved including evapotranspiration (Dutta et al., 2016b), ammonia volatilization (Congreves et al., 2016b; Dutta et al., 2016a), crop temperature stress and effects of CO_2 fertilization (Smith et al., 2013), impacts of snow and residue dynamics on soil temperature (Dutta et al., 2018) and inclusion of a winterkill sub-model (He et al., 2019a). Smith et al. (2019c), who compared Canada DNDC to RZWQM2 found limitations in simulating soil hydrology in DNDC and suggested several improvements including a deeper and heterogeneous soil profile, improved water flow down the profile, root density functions, a fluctuating water table and mechanistic tile drainage. In this study we incorporate these developments while attempting to minimize extra model inputs, complexity for users and computation time. In this study Canada DNDC prior to development is referred to as “default DNDC” and Canada DNDC post development is referred to as “revised DNDC”.

4.2.2.2 RZWQM2

RZWQM2 (version 3.0.2015; Ma et al., 2012) was developed to simulate detailed biogeochemical processes in cropping systems with a major focus on simulating water quality. The model simulates a wide array of agricultural management and has recently been expanded and improved for simulating N_2O emissions (Fang et al., 2012; Jiang et al., 2019) and phosphorous dynamics (Sadhukhan et al., 2019). RZWQM2 includes DSSAT 4.0 crop models with CERES and CROPGRO components (Hoogenboom et al., 2017; Ma et al., 2005, 2006) which is a very well established framework for simulating crop growth and development worldwide. RZWQM2 uses a numerical solution to determine water fluxes and includes the Green-Ampt equation for infiltration, the Richards equation with an option for lateral hydraulic gradient for lateral water loss, and the Hooghoudt’s equation for simulating quasi-2D tile drainage. Thus the model input requirements, modeller expertise and computation time are greater than for DNDC. The model has been validated for simulating drainage and N loading to tiles at many locations in North America (Malone et al., 2017; Xian et al., 2017; Qi et al., 2011b; Li et al., 2008; Thorp et al., 2007; Akhand et al., 2003) and has been employed to investigate BMPs for reducing N losses. Since RZWQM2 is a well-recognized model for simulating soil hydrology it offers an excellent opportunity for benchmarking DNDC developments.

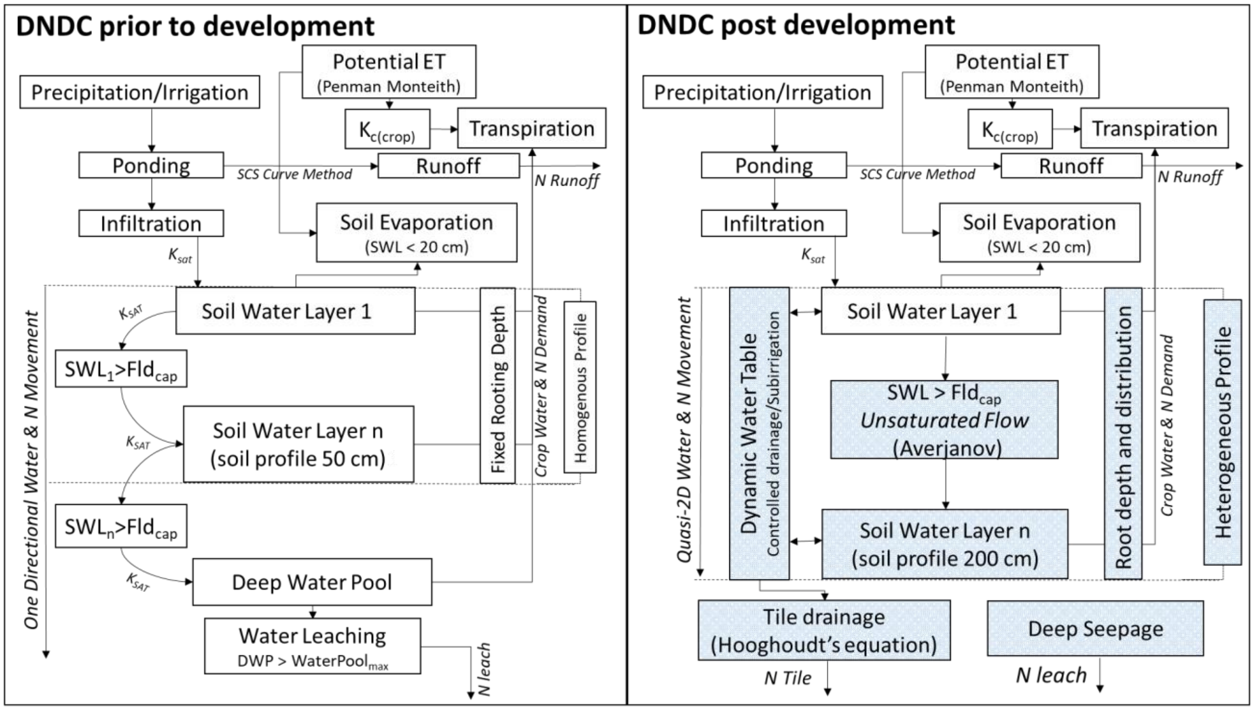

Figure 4.1 Schematic of Canada DNDC before and after development of improved hydrological processes. Shaded areas show which algorithms were modified. Revised model version available at https://github.com/BrianBGrant/DNDCv.CAN.

4.2.3 Development of DNDC to improve the simulation of soil hydrology and to include mechanistic tile drainage

4.2.3.1 Heterogeneous and deeper soil profile

The default DNDC model only characterizes the top soil horizon and assumes a homogeneous profile throughout. Often this is not a good representation of agricultural soils which can have striking differences across depths as a result of changing textures and organic carbon contents. Therefore, the model interface was restructured to allow for the user input of soil properties by definable layer depths. Soil properties that are now defined by depth include bulk density, soil organic carbon, pH, soil texture, field capacity, wilting point, porosity and saturated hydraulic conductivity. The user can specify the depth of the soil profile up to 200 cm and define properties for up to 10 user defined depths. The soil profile information can be saved such that it can be used for other simulations.

The modifications to the model interface were conducted in parallel with the model simulation depth being adjusted from 50 cm to 200 cm (Fig. 4.1). The total number of simulated layers were increased to ensure that the calculated layer thickness remained in the same range

(~0.5-2.5 cm) as it was previously for the 50 cm version of the model. This was important since many processes are formulated to calculate the mass and energy flows based on this conceptual range of layer thickness. It was decided that 200 cm would provide a sufficient depth to accommodate the effective root penetration of most commonly used crops and allow for the simulation of a fluctuating water table and tile drainage. Modifications to internal variables were conducted to ensure that soil properties, water, carbon, nutrients, and temperature could be tracked over the entire depth and these variables could be applied for estimating decomposition, denitrification, nitrification, fermentation, adsorption onto clay, chemical equilibria and N movement functions. As a result, DNDC was not only enhanced for simulating soil hydrology but also for the simulation of all biogeochemical processes up to a 200 cm depth.

4.2.3.2 Root penetration and density function

The default DNDC model calculates a linear estimate of root penetration to a maximum depth of only 50 cm, without considering root density. Since water uptake for transpiration is partitioned equally across the profile, this can result in the model underestimating water and N uptake near the surface and overestimating these components in the deeper profile. Further, crops only have access to 100 cm of soil water when the deep water pool is included (Fig. 4.1), thus deeper rooted crops can sometimes become water limited. As a result of these limitations in the default model, a root penetration equation based on growing degree days (GDD) (Pedersen et al., 2010) was incorporated into DNDC. Temperature or GDD are considered to be the main drivers for root growth and penetration (Kage et al., 2000; Thorup-Kristensen, 2006; Kirkegaard and Lilley, 2007). The equation, expressed in terms of PGI (Plant Growth Index) which is the fraction of accumulated degree days required for a plant to reach maturity in DNDC is as follows;

$$R_z = \begin{cases} R_{zmin} & ; PGI \leq PGI_{lag} \\ \sum\left(\left(PGI - PGI_{lag}\right)k_{rz}\right) + R_{zmin} & ; PGI > PGI_{lag} \\ R_{zmax} & ; PGI - PGI_{lag}k_{rz} + R_{zmin} > R_{zmax} \end{cases} \qquad (4.1)$$

where R_z is the depth of root penetration; R_{zmin} is the planting depth; PGI_{lag} accounts for the time period between planting and start of root penetration (germination); k_{rz} is the root depth penetration rate with values provided for some crops in Pedersen et al. (2010); R_{zmax} is the maximum root penetration depth. The R_{zmax} value is user defined in the DNDC input interface.

An algorithm for root distribution, based on a study by Gerwitz and Page (1974), and further modified by Yang et al. (2009) to extend the rooting depth of fine roots by an additional 30% was also employed in DNDC. The root density declines logarithmically to the root penetration depth (R_z) followed by a linear decrease to zero at $1.3R_z$. The relative root length distribution is as follows;

$$L_R(z) = \begin{cases} e^{-a_z z} & ;\ z < R_z \\ e^{-a_z z}\left(1 - \frac{z - R_z}{0.3R_z}\right) & ;\ R_z \leq z \leq 1.3R_z \end{cases} \tag{4.2}$$

where a_z is the shape parameter describing root distribution with increasing soil depth. Pedersen et al. (2010) used values of $a_z = 2$ for wheat and winter wheat and 1.5 for brassicas and we currently use a default value of 2 but the user can define the shape parameter and rooting depth based on field studies or from sources such as Fan et al. (2016) and Benjamin et al. (2013).

4.2.3.3 Simulating water flow

The default cascade flow algorithm, whereby water content per layer tips to field capacity on an hourly basis can result in an erroneously low prediction of soil water contents. Complex numerical schemes, such as finite difference and finite element solutions of Richards equation, can generally produce more accurate result; however, they are data and computation intensive. It is possible to use pedotransfer functions to estimate water retention curves and other hydrological parameters for use in these equations but in doing so it can undermine much of the improved accuracy that is achieved using this approach. Further, there is some uncertainty regarding the applicably of Richards equation for highly heterogeneous agricultural soils. In a review of water flow approaches, Beven and Germann (2013) commented that in unsaturated heterogeneous soils there is rarely a consistent hydraulic gradient, which Richards equation assumes, since capillary potentials are not in equilibrium.

Initially, we investigated including an integrated-Richards-equation approach with the van Genuchten equation (van Genuchten, 1980) for estimating soil water retention characteristics in DNDC, as presented in Yang et al. (2009) but once implemented, the hydrology sub-model time step needed to be reduced to such an extent that the computational time of DNDC was greatly increased and we also found it difficult to obtain data to properly fit the van Genuchten or other water retention equations. During the course of development, after the inclusion of a heterogeneous soil profile, root density function and mechanistic tile drainage, we found that the cascade approach could provide sufficient accuracy in estimating water contents/flux. We decided to keep the cascade flow approach intact but limited water movement above field capacity based on soil water status using the following simple approach derived by both Averkjanov (1950) and Irmay (1954) for estimating unsaturated conductivity.

$$K = K_{SAT}\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^n \qquad (4.3)$$

where K is hydraulic conductivity, K_{SAT} is saturated hydraulic conductivity, θ is actual, θ_r residual, and θ_s saturated soil water content ($cm^3\ cm^{-3}$). This equation differs in power (n) where Irmay used a value of 3 and Averkjanov 3.5. Our tests indicate that a value of 3.5 worked well in the range of soil water contents from field capacity to saturation, the only incidence when K is calculated in revised DNDC.

4.2.3.4 Fluctuating water table

DNDC was modified to simulate a fluctuating water table by adjusting the hydraulic conductivity of the deepest profile to near impermeable (user defined value). A water table slowly builds up from the bottom soil layer with deep seepage at the lower boundary. The water table is maintained as a mass balance of incoming water from precipitation and irrigation and outgoing water from runoff, evapotranspiration, tile drainage, deep seepage and change in soil water content in unsaturated layers. For the purposes of estimating tile flow rate, the water table height was calculated at the top of the saturated soil layer closest to the soil surface.

4.2.3.5 Incorporate a tile drainage sub-model

Similar to RZWQM2 and DRAINMOD (Skaggs et al., 2012), the steady state Hooghoudt equation was also included in DNDC. The drawdown of water table height is not fully steady state, however, the rate of change usually proceeds slow enough that the Hooghoudt equation can be used effectively (Skaggs et al., 2012). A recent study by Xian et al. (2017), when assessing the performance of RZWQM2 using the original steady state equation and two transient equations, found that there was no significant difference in model performance for hourly drainage simulation. The Hooghoudt equation as written in Skaggs et al. (2012) is;

$$q = \frac{4K_e m(2d_e+m)}{L^2} \tag{4.4}$$

where q (cm h^{-1}) is the drainage discharge rate, K_e (cm h^{-1}) is the effective lateral hydraulic conductivity, m is the water table level above the drain at midpoint between the drains, d_e is the equivalent depth to the impermeable (or restrictive) layer below the drain, and L is the drain spacing. Equations to estimate K_e and d_e below were outlined in Xian et al. (2017).

$$K_e = \frac{\int_{i=1}^{i=n} D_i K_i}{\int_{i=1}^{i=n} D_i} \tag{4.5}$$

where n is the number of soil layers, D_i is the thickness of layer i (cm), and K_i is the lateral hydraulic conductivity of layer i (cm h^{-1}).

The calculation of de depends on the actual depth (d) of the soil profile:

$$\text{if} \quad \frac{d}{L} < 0.3 \qquad d_e = \frac{d}{1+\frac{d}{L}\left[\left(\frac{8}{\pi} ln\frac{d}{r}\right) - CON\right]} \tag{4.6}$$

$$\text{where} \quad CON = 3.55 - 1.6\frac{d}{L} + 2\left(\frac{d}{L}\right)^2 \tag{4.7}$$

$$\text{if} \quad \frac{d}{L} \geq 0.3 \qquad d_e = \frac{L}{\left(\frac{8}{\pi} ln\frac{L}{r}\right) - 1.15} \tag{4.8}$$

where r is the radius of the drain (m).

The ability to simulate controlled drainage was implemented in the model by allowing the user to set an effective depth of drainage below the soil surface. An unlimited number of sub-irrigation and controlled drainage events can be set, with starting and end days for each event, in the “irrigation” tab of the model interface. For each sub-irrigation event the quantity of water applied and number of irrigation days can be set.

4.2.3.6 Movement of nitrogen to runoff, tile drains and through the soil profile

The primary development aim of this study was to improve estimation of soil hydrology and thus the existing N movement mechanisms in DNDC were not extensively modified. The default nitrate movement in DNDC is described simply as a function of the water flux and nitrate concentration per layer. Soil nitrate was considered to be mobilized by a positive water flux (90% mobilized) and transferred to the layer below as a one-dimensional vertical N flux towards the bottom soil profile. Additionally, another fraction (10% of the NO_3^- in a layer) was considered to be lost through preferential water flow via macropores directly out of the soil profile. This preferential loss was calculated regardless of whether the soil layer directly below also met the condition of having a positive water flux.

For simulations now with tile drainage, the movement of nitrate is an iterative step through each of the saturated layers per hour that are drained to tiles. In DNDCv.CAN this preferential N loss function was modified to ensure correlation with water movement. It was previously found that DNDC sometimes simulated N losses when there was no water flux out of the bottom of the soil profile. In DNDCv.CAN the fraction of NO_3^- available to be transferred to the layer below at an hourly time step can now be parameterized through the user interface with a default value of 0.9. The fraction per layer that is preferentially lost directly to drains (i.e. it bypasses the iterative layer loop) is set to a default fraction of 0.02. Nitrate losses to tile drains are calculated starting from the layer situated at the top of the saturated water table down to the layer at the bottom of the tile drains.

Additionally, we found that default DNDC nitrate losses to runoff were always very low, irrespective of the crop management system that was employed. To address this issue we first fixed a water mass balance error in the SCS runoff curve number method. Second, the model was modified to simulate a fluctuating water table and when the water table reaches the soil surface runoff and additional loss of N could then occur. Further, N loss to runoff was originally calculated as a fraction of rainfall that goes to runoff (based on SCS method) multiplied by the nitrate found in only the top surface layer (~0.5 - 2 cm). We extended this calculation to the top 2 layers and included a user defined parameter where the fraction can be adjusted.

4.2.4 Initialization, calibration and validation

At both the Gilmore City and Woodslee research locations the TD-CC-MS treatment was used for model calibration and the remaining 3 treatments were used for validation. A similar trial and error method for calibration as conducted in Smith et al. (2019c) was used where the RMSE for simulated yield, drainage and N loss to tiles was minimized. This was conducted for default DNDC, revised DNDC and RZWQM2. In all simulations, a 10 year spin-up was included prior to the experimental periods to stabilize soil C, N and water.

Experimental data from the sites was used to initialize the models. This data included soil properties, such as soil texture, bulk density, field capacity, wilting point, porosity, saturated hydraulic conductivity and soil organic carbon content (Table 4.S1). Note that soils data was only available at two depths at the Woodslee site, thus the properties from the 10-20 cm depth were extrapolated down to 200 cm. Daily weather data, including min and max temperature, precipitation, wind speed, solar radiation and relative humidity, were available at both sites for all years of the studies. Management data, including tillage scheduling and implements and fertilizer scheduling and application rates, was also available.

For the Gilmore City site, default DNDC and RZWQM2 have previously been calibrated and validated (Smith et al., 2019c). In this study we compare the performance of the revised DNDC model to those results. After the hydrology developments had been implemented, the revised model was calibrated using the same approach as the other two models. Crop, soil and tile drainage parameters used in the study for default and revised DNDC are shown in Table 4.S2 and crop parameters used in RZWQM2 are shown in Table 4.S3. Note that a winter rye cultivar was not available in RZWQM2, thus Qi et al. (2011b) developed parameters based on a winter wheat cultivar and these were further modified for a more recent version of RZWQM2 by Smith et al. (2019c).

4.2.4.1 Calibration of crop parameters in DNDC

For revised DNDC, several crop parameters were calibrated however parameters remained close to those used by default DNDC. The thermal degree days to maturity (TDD) was increased marginally for both maize and soybean (Table 4.S2). Water requirement for maize and soybean were reduced. At Gilmore City, soybean was set to 340 which is very close to the default 350 value for the U.S. release version. In default DNDC plant roots only had access to the top 100 cm of the profile and had no access to a water table. The crop water requirement was increased in order to simulate an appropriate level of crop water uptake, evapotranspiration and drainage which often resulted in soil water content that was too low in the growing season (Smith et al., 2019c). In the revised DNDC model, these crop water requirements were calibrated to be on average 15% lower for maize and 23% lower for soybean.

At the Woodslee location the average soybean yields were only 60% of that at Gilmore City. We believe this was partly due to different varieties being used than at Gilmore City (a different variety was planted every year at Woodlsee as the soybean variety A2553 was no longer available in 2005 and a shorter-season variety was planted in 2003 as a result of a late plant date: Drury et al., 2014b). We used a lower maximum grain C parameter (optimum yield) at Woodslee for soybean (Table 4.2). However, the main contributing factor was likely that more crop water stress occurred at Woodslee. This was attributed to greater runoff due to a lower permeability soil and more precipitation occurring in the off-season months. Also, Woodslee receives less average precipitation, during the growing season than at Gilmore City (Fig. 4.S1).

In default DNDC, rooting depth is always constant at 50 cm. In revised DNDC we set a lower max root depth at Woodslee site since there is higher clay content and lower root penetration (Table 4.S2). This helped minimize RMSE for yields and drainage. Rooting depth in DNDC was set considerably lower than in RZWQM2 which has max possible root depth of 1.8m for both maize and soybean.

For the winter-rye cover crop at Gilmore City, the parameters used in Smith et al., (2019c) for default DNDC were employed for revised DNDC. Default parameters for both default and revised DNDC were used for the winter wheat cover crop grown at the Woodslee site. The winter rye and winter wheat cover crop never reached the grain filling stage before being terminated in any of the treatments simulated. A similar magnitude of winter wheat biomass was simulated for DNDC and RZWQM2 at Woodslee but no measured data was available for validation.

4.2.4.2 Calibration of soil and drainage parameters in DNDC

The drainage development required the integration of additional input parameters to the DNDC interface including drain depth, spacing and radius, depth to bedrock, and K_{SAT} at each depth. Lateral K_{SAT} is estimated as 2*K_{SAT} (Qi et al., 2011b) which is needed to calculate K_e for use in the Hooghoudt equation. In general, it is very difficult to get a good measure of *in situ* K_{SAT}, particularly at deeper soil depths. Laboratory measurements of K_{SAT} using soil cores and the traditional saturated flow-desorption method can in fact be over an order of magnitude greater than *in situ* measured K_{SAT} (Smith et al., 1995). In this this study we used the K_{SAT} values from Qi et al. (2011b) for the Gilmore City site and adjusted K_{SAT} with depth for the Woodslee site to values that would provide a good estimate of tile drainage using both DNDC and RZWQM2 (Table 4.S1)

During the calibration process for default DNDC, it was necessary to reduce the size of the slow humus soil organic carbon (SOC) pool from a default value of 0.95 to 0.7 to provide sufficient N mineralization when simulating the observed levels of N losses at the Gilmore City site (Smith et al., 2019c). Using revised DNDC it was only necessary to reduce this parameter to 0.90. The revised DNDC model simulates decomposition to 200 cm and thus it estimates a more plausible rate of mineralization, which was previously noted to be a model weakness in some studies (Grant et al., 2016; Smith et al., 2008). Similar to the Gilmore City location, for default DNDC it was necessary to reduce the size of the slow humus SOC pool in default DNDC from 0.95 to 0.75 to simulate the correct magnitude of N losses in the calibration treatment at Woodslee. Using revised DNDC this value was decreased only to 0.91. The SCS curves number for estimating runoff in revised DNDC at Gilmore City was set to 64, the same value as used for default DNDC (Smith et al., 2019c). A value of 87 was used at Woodslee for both model versions to account for a lower permeability soil and thus simulate the correct level of runoff for the calibration treatment. Preferential movement of N was set to 2% in revised DNDC to allow rapid movement of a small portion of N to drains, without moving through the soil matrix. This improved the model performance at both sites.

The N concentration in precipitation was set to 1.8 mg N L^{-1}, the same value as used at the Gilmore City site (Qi et al., 2011b). The microbial parameters related to nitrification and denitrification rates were left as default, however, during the course of development we added several new parameters into the DNDC input interface such that they could potentially be adjusted. The rate of microbial activity can vary greatly between soil types and locations.

4.2.4.3 Calibration of RZWQM2 at Woodslee site

A similar procedure employed in Smith et al. (2019c) and Qi et al. (2011b) at the Gilmore City site was used for calibrating RZWQM2 at the Woodslee site. Measured soil properties were input into the model according to Table 4.S1. Initial soil moisture was set to saturation below the 60 cm depth at the beginning of the 10 year spin-up to initiate the simulation of a water table. The magnitude of the initial soil carbon was based on site measurements, however, the partitioning of the SOC pools was determined by using a built in tool for equilibrating SOC based on total SOC at the soil surface, global position and regional temperatures. Similar to Smith et al. (2019c) at the Gilmore City site it was necessary to increase the decomposition rate of the SOC pools by about 30% at the Woodslee site in order to simulate the appropriate level of N mineralization and subsequent N losses to tile drainage and runoff. The simulated organic N levels in the soil profile remained stable over the five year study. The N concentration in precipitation was set to the same total N input rate as for DNDC with values of 0.5 mg N L^{-1} and 1.3 mg N L^{-1} for NH_4^+, and NO_3^- respectively.

The impermeable layer was set at 390 cm with a K_{SAT} rate of 0.01 cm h^{-1} in the bottom layer which limited flow and maintained a water table. The Brookes-Corey soil water retention model was used with curve fitting parameters being estimated internally in RZWQM2 based on measured water contents at saturation, 1/10 bar, 1/3 bar and 15 bar (wilting point).

Similar to DNDC, the crop parameters in RZWQM2 needed to be lowered to simulate the appropriate level of crop yields at the Woodslee location, particularly for soybean. A number of the DSSAT crop parameters for maize (IB 1068 Dekalb 521) and soybean (990002 M Group 2) were left as default, particularly the ones controlling phenology, however, to optimize RMSE for biomass for the calibration treatment at Woodslee we reduced three crop parameters for maize and five parameters for soybean (Table 4.S3). Default parameters for winter wheat (990003 winter-US) were used at Woodslee.

4.2.5 Statistical measures for testing model performance

Model performance of default DNDC, revised DNDC and RZWQM2 were evaluated using several statistical measures including normalized average relative error (NARE; %), normalized root mean square error (NRMSE; %), Nash-Sutcliffe model efficiency coefficient (NSE; Nash and Sutcliffe, 1970) and the d index (Wilmott and Matsuura, 2005).

$$NARE = 100\left(\frac{\frac{1}{n}\sum_{i=1}^{n}(P_i - O_i)}{\bar{O}}\right) \tag{4.9}$$

$$NRMSE = 100\left(\frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(O_i - P_i)^2}}{\bar{O}}\right) \tag{4.10}$$

$$NSE = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \tag{4.11}$$

$$\mathrm{d} = 1 - \frac{\sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(|P_i - \bar{O}| + |O_i - \bar{O}|)^2} \tag{4.12}$$

where P_i is the predicted or simulated value and O_i is the observed value.

NARE is the average percent over- or under-prediction of a model relative to measurements. Both NRMSE and NARE are commonly used to evaluate model performance for estimating yield and biomass. Jamieson et al. (1991) indicated that a model had excellent performance if NRSME < 10; good < 20; fair < 30; and poor > 30 whereas Ahuja et al. (2000) indicated satisfactory performance if NARE < 15% for estimating yield and biomass.

NSE and d statistics are commonly employed for estimating water and N leaching and runoff. An NSE value of greater than 0 for NSE indicates the model estimates are more accurate than the average of observations. NSE has a maximum value of 1 and a negative NSE indicates poor model performance. However, NSE is more sensitive to values that have higher deviation (Kraus et al., 2005) and may in certain instances be close to zero or negative even when model results are very close to measurements (but the measurements show little deviation), thus it is important to also assess NARE and NRMSE. The d index provides a qualitative assessment of model accuracy with $d \geq 0.9$ showing an "excellent" agreement between model and observed values, $0.8 \leq d \leq 0.9$ indicates a "good" agreement, $0.7 \leq d \leq 0.8$ a "fair" agreement and $d < 0.7$ a "poor" agreement. For water drainage and N flow to tiles Moriasi et al. (2007) considered model performance to be satisfactory if NSE > 0.5. Drainage was satisfactory if NARE < 25% and N loss to tiles if NARE < 70%.

4.3 Results and discussion

It was previously demonstrated that the default version of Canada DNDC performed well for simulating crop yields, monthly water and N loss to tile drains at the Gilmore City (Smith et al., 2019c). In this study we verified that the revised model performed well for these components, however, most of the emphasis was placed on testing the model for simulating soil water storage and daily N and water loss to tile drains at Gilmore City, for which it did not previously perform well and also for simulating drainage and runoff at the Woodslee site. In addition we tested the new functionality of the model for simulating controlled drainage and sub-irrigation.

4.3.1 Simulation of crop yields

The revised DNDC model performed well in simulating crop yields at the Gilmore City site giving similar results as both the previously tested models, default DNDC and RZWQM2, as reported by Smith et al. (2019c). All three models demonstrated good to excellent performance (NRMSE < 20%) for yield estimates except for soybeans in the TD-CC-SM treatment which were over-predicted in 2007 and 2009 (Table 4.4). These were years which had lower seasonal GDD, perhaps supressing observed yields. Data from only 2006 and 2008 (Table 4.2) were used to calibrate both models thus the temperature stresses imposed by a shorter growing season may not have been well characterized. It was interesting that the improvements to hydrology simulation, as will be demonstrated in subsequent sections, did not improve yield prediction for this site with average statistic being similarly good between models. The RMSE levels in this study were generally lower than those in Jerecki et al. (2018) where the estimates for maize were over 1100 kg DM ha^{-1} using DNDC.vCan.

At the Woodslee location, all models demonstrated good to excellent performance (NRMSE's < 20%) for simulating maize and soybean yields under the unrestricted tile drainage calibration and validation treatments. Note that revised DNDC performed better than default DNDC for maize and large improvements were observed for soybean likely as a result of the improved hydrology simulation. Crops are generally more water limited at Woodslee due to more off-season runoff and less growing season precipitation. Maize yields were also well simulated by both revised DNDC and RZWQM2 for both the CC and NCC treatments under CDS. Of course, default DNDC was not capable of simulating controlled drainage or sub-irrigation. Both DNDC and RZWQM2 showed fair performance in simulating soybean yield under CDS-CC but interestingly their performance was poor for CDS-NCC with about a 40% overestimation of yields. Revised DNDC produced similar NRMSE values as RZWQM2, demonstrating the value of running more than one model for a study. Both models simulated less crop water stress in this system with controlled drainage and sub-irrigation. In investigating measurements, the observed drainage volumes are reduced for the controlled drainage systems relative to the unrestricted drainage for both CC and NCC treatments. This difference may have been greater if sub-irrigation was not applied. The CDS-NCC system appears to have behaved counterintuitive to what might have been expected since observed overall runoff + drainage to tiles was about 10% less than the other 3 treatments (Table 4.S4), yet crop yields (and assumedly evapotranspiration) were similar. One explanation is that there may have been more deep seepage for this plot which is further discussed in subsequent sections.

Table 4.4 Statistical performance of models for simulation crop yields at Gilmore City and Woodslee

Treatment	Crop	Default* DNDCv.CAN NARE	Default* DNDCv.CAN RMSE (kg DM ha⁻¹)	Default* DNDCv.CAN NRMSE	Revised DNDCv.CAN NARE	Revised DNDCv.CAN RMSE (kg DM ha⁻¹)	Revised DNDCv.CAN NRMSE	RZWQM2* NARE	RZWQM2* RMSE (kg DM ha⁻¹)	RZWQM2* NRMSE
Gilmore City										
TD-CC-MS#	Maize	7.3	1028	12.8	4.8	1284	16.0	0.4	1337	16.7
TD-NCC-MS	Maize	1.7	962	11.4	0.6	1133	13.4	-4.0	1184	14.0
TD-CC-SM	Maize	-4.6	852	9.6	2.3	679	7.7	0.9	236	2.7
TD-NCC-SM	Maize	-8.7	818	8.9	-5.7	559	6.1	1.7	509	5.5
TD-CC-MS#	Soybean	0.2	171	5.9	-0.9	215	7.4	2.2	63	2.2
TD-NCC-MS	Soybean	-8.9	377	12.0	-8.8	382	12.1	-5.5	181	5.8
TD-CC-SM	Soybean	13.7	575	22.3	13.4	586	22.8	14.0	538	20.9
TD-NCC-SM	Soybean	10.1	425	16.0	8.8	376	14.2	12.1	348	12.1
Woodslee										
TD-CC-MS#	Maize	2.6	1152	15.9	-6.7	694	9.6	0.8	978	13.5
TD-NCC-MS	Maize	2.0	798	10.8	-7.2	778	10.5	-4.8	735	10.0
CDS-CC-MS	Maize	NA	NA	NA	11.4	834	11.6	5.5	597	8.3
CDS-NCC-MS	Maize	NA	NA	NA	13.4	974	13.8	7.5	781	11.1
TD-CC-MS#	Soybean	-2.0	328	17.3	-4.9	156	8.2	-1.1	330	17.4
TD-NCC-MS	Soybean	1.0	280	15.9	3.1	127	7.2	7.1	339	19.3
CDS-CC-MS	Soybean	NA	NA	NA	17.0	421	21.8	4.9	420	21.7
CDS-NCC-MS	Soybean	NA	NA	NA	38.5	675	40.1	41.7	767	45.6

*Simulations for default Canada DNDC and RZWQM2 at Gilmore City site were performed by Smith et al. (2019)
#Calibration treatment

4.3.2 Soil water storage at Gilmore City

As demonstrated by Smith et al. (2019c) soil water storage was poorly simulated by default DNDC and reasonably simulated by RZWQM2. This was the case across all four treatments. Some of the main issues were that DNDC did not include root density functions, a heterogeneous profile or unsaturated flow. During this development, we found that characterizing these aspects improved the model, particularly the addition of root density functions. Higher root density near the soil surface resulted in more water uptake near the soil surface (Fig. 4.2; 0-6 cm depth) thereby improving the water content simulation. However, the largest improvement for simulating soil water content resulted from the inclusion of a fluctuating water table and mechanistic tile drainage. Default DNDC greatly under predicted soil water storage at deeper depths in the summer months primarily because crop roots had no access to the water table. Post-development, the roots could now penetrate beyond 50 cm to a depth defined by the user, with fine roots penetrating 30% further, and potentially allowing plant roots to access the water table. This greatly improved the model fit for simulating soil water content at deeper depths (Fig. 4.2) and soil water storage to 60 cm depth (Fig. 4.3). As demonstrated by the statistical performance (NSE and d) of default and revised DNDC (Table 4.5) soil water storage was improved for all treatments from fair/poor ($0.69 \leq d \leq 0.79$) performance to good/excellent ($0.81 \leq d \leq 0.90$) performance. All three models predicted the average magnitude of soil water content well during the 5 year study ($-1.3 \leq NARE \leq 4.6$), however, revised DNDC and RZWQM2 performed much better in predicting the trends over time. Revised DNDC had similar performance as RZWQM2 for the CC treatments and had improved performance for the NCC treatments. Interestingly, the soil water storage as predicted by RZWQM2 indicated that drainage from the profile was sometimes more delayed in relation to observations. This may be related to an issue with using Richards equation since it assumes a consistent hydraulic gradient which often does not exist in heterogeneous agricultural soils (Beven and Germann, 2013). This limitation is partly overcome in RZWQM2 by discretizing the heterogeneous soil profile into layers. Note that Berninger et al. (2015) derived a method for multidomain discretization and found that the approach was reasonably robust but it sometimes suffered from lack of discrete local mass-conservation.

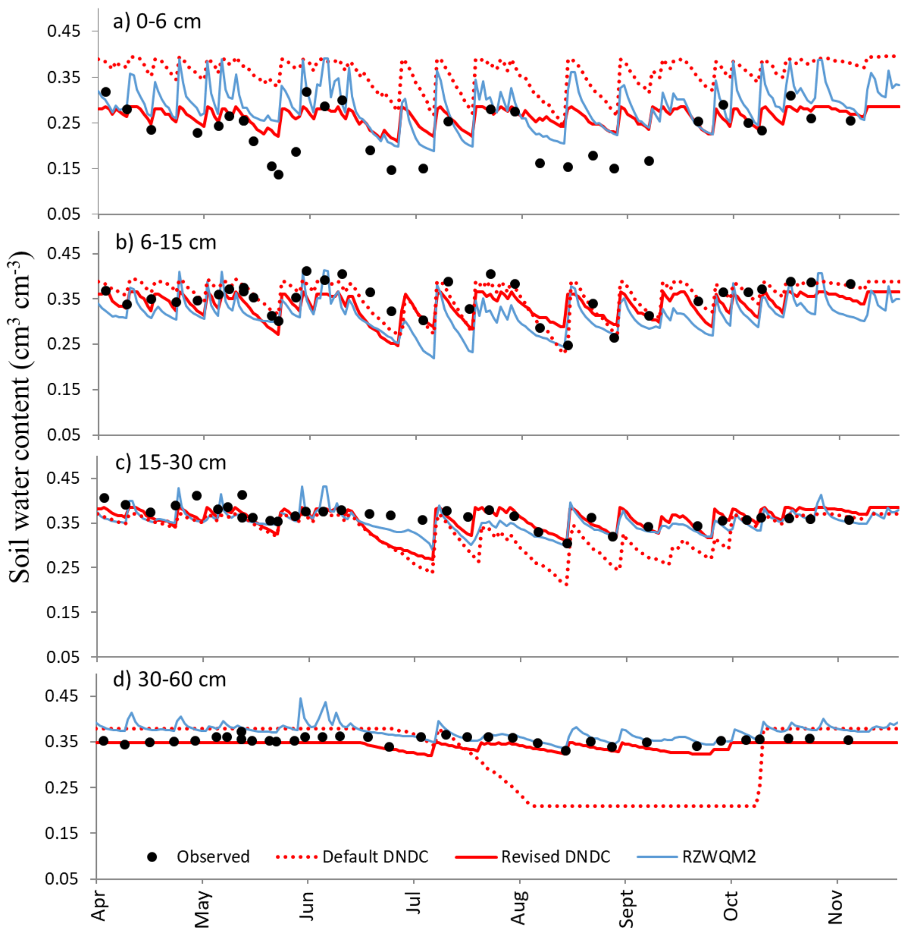

Figure 4.2 Observed and simulated soil water content by depth in 2008 for validation treatment TD-CC-SM at Gilmore City

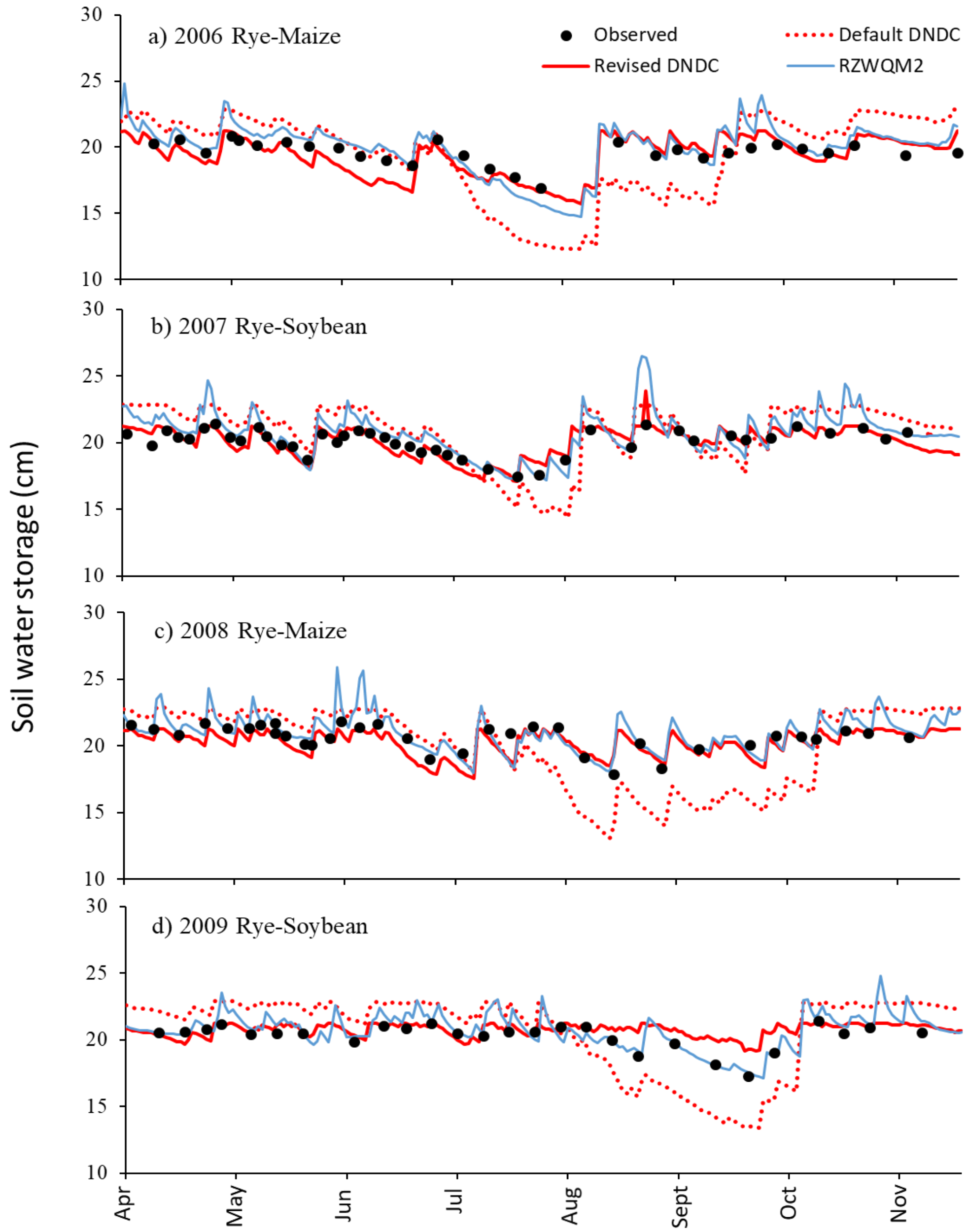

Figure 4.3 Observed and simulated soil water storage to 60 cm depth for validation treatment TD-CC-SM at Gilmore City

Table 4.5 Statistical performance of models for simulating drainage and N loss to tile drains at the Gilmore City research site

		Calibration			Validation								
		TD-CC-MS*			TD-NCC-MS			TD-CC-SM			TD-NCC-SM		
Water/N component	Statistic	Default DNDC	Revised DNDC	RZWQM	Default DNDC	Revised DNDC	RZWQM	Default DNDC	Revised DNDC	RZWQM	Default DNDC	Revised DNDC	RZWQM
Soil water storage (0-60 cm depth)	NARE	1.9	-1.3	1.1	4.6	1.7	4.3	0.8	-0.6	1.9	2.8	1.1	4.5
	NSE	-1.05	0.41	0.46	-4.52	0.11	-0.52	-3.61	0.35	0.08	-1.18	0.46	-0.03
	d	0.79	0.88	0.87	0.69	0.81	0.76	0.72	0.84	0.84	0.74	0.90	0.77
Tile drainage (monthly, 2005-2009)	NARE	1.6	3.9	6.0	-5.3	-0.8	-1.4	-16.1	-15.2	-13.3	17.5	16.0	24.5
	NSE	0.73	0.69	0.67	0.71	0.74	0.76	0.65	0.72	0.65	0.62	0.72	0.60
	d	0.92	0.90	0.90	0.91	0.92	0.92	0.87	0.90	0.87	0.90	0.93	0.90
Tile drainage (daily, 2007-2008)	NARE	-2.6	-6.9	3.2	-10.3	-13.7	-9.2	-22.9	-20.2	-18.5	8.2	3.1	14.5
	NSE	-0.32	0.55	0.35	0.08	0.51	0.50	0.24	0.60	0.50	-0.11	0.70	0.69
	d	0.68	0.80	0.76	0.71	0.76	0.79	0.74	0.81	0.77	0.67	0.88	0.90
N loss to tiles (monthly, 2005-2009)	NARE	7.4	8.9	0.2	-3.0	-4.6	-1.4	-10.7	-3.1	-17.8	14.1	11.7	13.7
	NSE	0.53	0.69	0.67	0.65	0.77	0.67	0.59	0.75	0.51	0.58	0.64	0.44
	d	0.85	0.92	0.89	0.89	0.93	0.91	0.83	0.93	0.82	0.86	0.92	0.86

* TD – unrestricted tile drainage; CDS – controlled drainage and subsurface irrigation; CC – cover crop; NCC – No cover crop; MS - Maize-soybean rotation phase; SM – Soybean-maize rotation phase

4.3.3 Tile drainage at Gilmore City

The implementation of a water table, mechanistic tile drainage and root penetration functions in DNDC resulted in the simulation of a fluctuating water table that was distinctly similar to RZWQM2 (Fig. 4.S2). A similar level of water table draw down during the growing season occurred each year, due to crop water uptake (transpiration) and also the rise in water table after rainfall events and the time required for drainage to the tile depth were similar. As a result the simulated daily water flow to tile drains was often remarkably similar as is demonstrated in validation treatment TD-CC-SM (Fig. 4.4). The daily predicted drainage flows for revised DNDC and RZWQM2 often overlapped. We found that the inclusion of Hooghoudt's equation was particularly crucial for simulating the correct timing of events, which gave DNDC the same functionality of commonly used water quality models such as RZWQM2 and DRAINMOD (Skaggs et al., 2012). Default DNDC, which simulates bulk flux of water down the profile via the cascade approach, simulated peak flow events that were too high and diminished too quickly, however, monthly flow was well simulated (Table 4.5).

Revised DNDC demonstrated excellent performance (d ≥ 0.90; NSE ≥ 0.69) for simulating monthly water flow to tile drains for the three validation treatments, with marginal improvements over default DNDC, which was previously found to perform well for monthly flow (Smith et al., 2019c) (Table 4.5). All three models predicted the correct average magnitude of drainage from TD-CC-MS and TD-NCC-MS treatments but under-predicted the drainage from treatment TD-CC-SM and over-predicted it from TD-NCC-SM. Observations indicated that more loss occurred to tile drains from TD-CC-SM (with cover crop; 347 mm over 5 years) than TD-NCC-SM (without cover crop; 252 mm over 5 years) which is unexpected. This disparity may be attributed to measurement variability during peak flow events in 2007 and 2008 which were high (Smith et al., 2019c). This variability was not taken into account in the model performance statistics. All three models predicted more transpiration and less water loss to tile drains in treatments with cover crops than without. Experimental studies generally report no difference in subsurface drainage (Drury et al., 2014b; Qi et al., 2011a; Qi et al., 2011c; Kaspar et al., 2007) or reduced drainage (Qi and Helmers, 2010; Strock et al., 2004) when a cover crop was present. The performance of revised DNDC for simulating daily drainage was improved in all treatments, particularly for TD-CC-MS and TD-NCC-SM where NSE values went from negative (worse than the average of measurements) to > 0.5 (Table 4.5). Note that daily measurements were only available in 2007 and 2008 (Qi et al., 2011b). The d statistic indicated that simulations changed from being characterized as poor to fair (i.e. d from 0.68 to 0.74) to fair to good (i.e. 0.76 to 0.88). Average statistics across treatments were similar between revised DNDC and RZWQM2 indicating that developments were successfully implemented. In particular, we found that the inclusion of mechanistic tile drainage improved the performance of revised DNDC, which is consistent with David et al. (2009) who found that models designed to simulate tile drainage (SWAT, EPIC and Drainmod-N), performed better for simulating bulk water flux than those which did not (DayCent, DNDCv.82a and DNDCv.82h). Malone et al. (2017) compared the performance of the HERMES model to RZWQM2 for simulating water and N loss to tile drains. The HERMES model, which did not include mechanistic drainage, performed reasonably well but RZWQM2 performed better in simulating monthly drainage. Guest et al. (2017a) found that Canada DNDC performed similarly to DayCent and STICS models for simulating soil water dynamics, but the three models all included cascade water flux approaches at the time. In a cross-Canada assessment Guest et al. (2018) found that Canada DNDC performed a little better than the water budget models VSMB and HOLOS, but the water budget models did not explicitly simulate crop water stress and the feedbacks from crop growth and development.

The revised DNDC improved the simulation of monthly N loss to tile drains, demonstrating excellent performance across all treatments, with better NSE and d statistics than both default DNDC and RZWQM2. Note that N concentrations in tile drainage were measured less frequently than water volumes (Qi et al., 2011b). Similar to water flow, all 3 models under-predicted N loss for the TD-CC-SM treatment and over-predicted for the TD-NCC-SM treatment. However, similar to the models, most studies show reduced N loss to tiles when a cover crop was included (Malone et al., 2017; Drury et al, 2014b; Li et al., 2008; Kaspar et al., 2007; Parkin et al., 2006; Strock et al., 2004). At the Gilmore City site the difference in N loss between the treatments, based on observations, was not found to be significant (Qi et al., 2011a) and thus the higher average annual loss from TD-CC-SM (39.9 kg ha^{-1} y^{-1}) relative to TD-NCC-SM (33.7 kg ha^{-1} y^{-1}) may be related to measurement variability.

Most of the development in this study focused on improving soil hydrology and drainage, however, we still found it necessary to adjust the way N moved and was simulated in DNDC (both U.S. DNDC and DNDCv.CAN). The model was adjusted to simulate N loss to tiles at the depth of the drains, but also to only allow preferential N movement to occur when there was water movement. This improved the timing of simulated N loss events, as is demonstrated for validation treatment TD-NCC-MS in Fig. 4.5. Although the simulated upper soil profile was frozen and there was no water movement in the fall and winter of 2005, N loss to tiles was still simulated using default DNDC. Note that the magnitude of cumulative N loss to tiles was initially underestimated by the revised model, but the timing of events was better simulated. Simulating preferential N movement as a function of water flow, the implementation of N loss to drains at the specified depth, and improved simulation of hydrology were responsible for the improved statistics noted in Table 4.5.

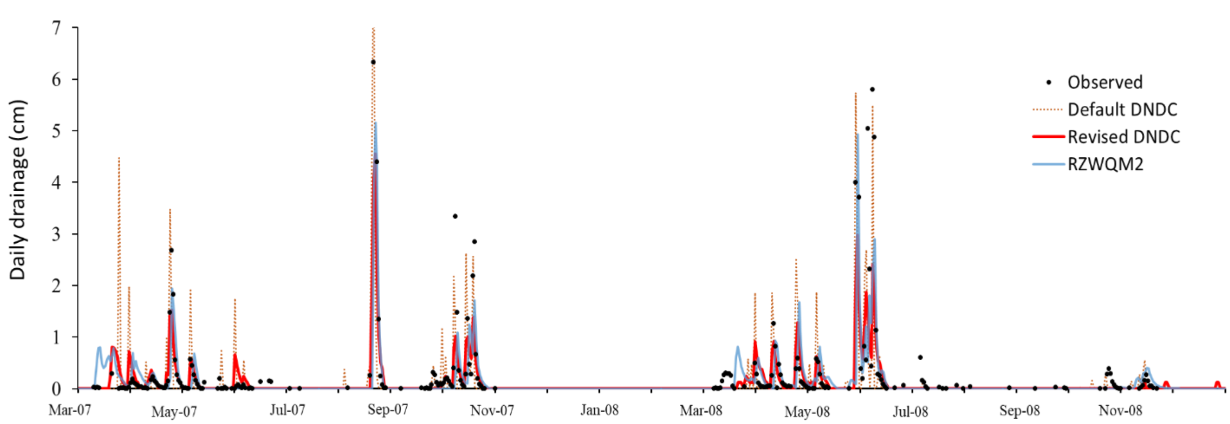

Figure 4.4 Observed and simulated daily water flow to tile drains for validation treatment TD-CC-SM at Gilmore City from 2007 to 2008

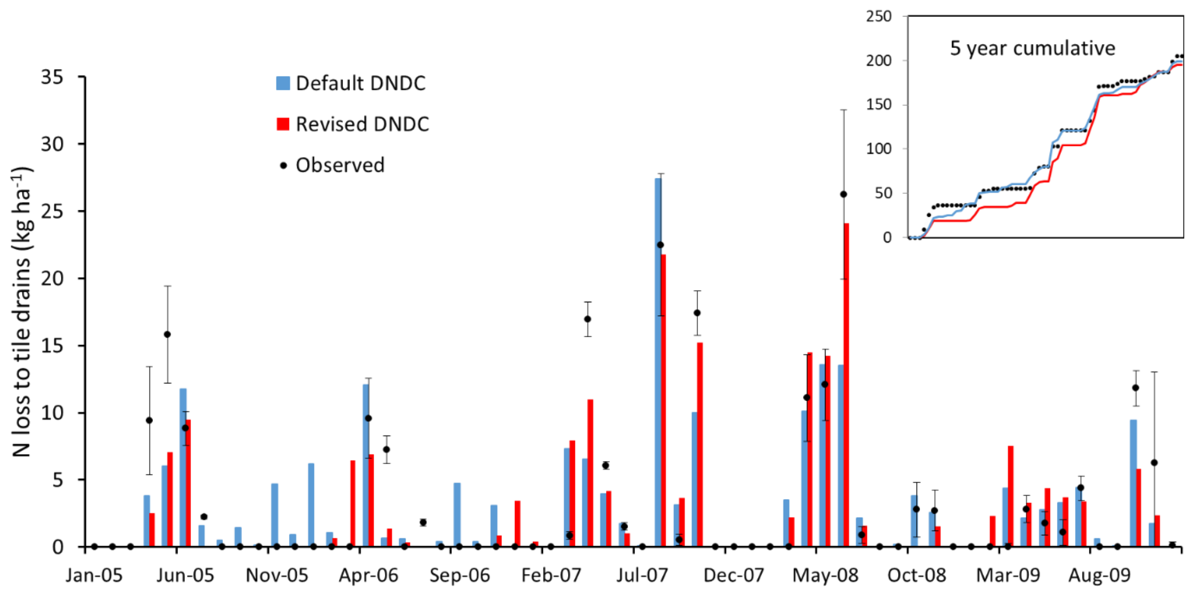

Figure 4.5 Comparison of monthly simulated N loading to tiles using default and revised DNDC for the TD-NCC-MS validation treatment at Gilmore City

4.3.4 Runoff and tile drainage at Woodslee

Although soil water contents were not available at the Woodslee site, there was an opportunity to benchmark the simulation of water and N loss to runoff along with the implementation of controlled drainage and sub-irrigation for DNDC. In general, the revised DNDC model demonstrated "good" to "excellent" performance ($0.83 \leq d \leq 0.96$; Table 4.6; Fig. 4.6) for simulating tile drainage for the validation treatments, with notable improvement over default DNDC ($d \leq 0.68$; "poor" performance) for the unrestricted tile drainage treatments. Default DNDC does not have the capability of simulating controlled drainage or sub-irrigation and thus could not be evaluated for these aspects. RZWQM2 showed "good" performance across all treatments, which was certainly satisfactory but could perhaps have been improved if additional measured soil hydraulic properties were available below 20 cm depth at the site. RZWQM2 uses the Brooks-Corey four parameter nonlinear curve fitting model for fitting water retention data and a better fit can be provided if measured saturated and residual soil water contents, pore size distribution and bubbling pressure are available. Even though revised DNDC and RZWQM2 demonstrated "good" performance in simulating drainage events, according to the d statistic, the overall magnitude of drainage was well simulated for only 3 of the treatments. For the CDS-NCC-MS treatment, observed water losses from runoff + tile drainage were considerably lower (Table 4.S4) than for the other three treatments. Evapotranspiration was not measured but it's unlikely that there was more water loss due to ET since observed yields were similar between treatments. It is possible that there was more deep seepage, but we did not have available soil physical and hydraulic properties at deeper depths and deep seepage was assumed to be minimal (which resulted in good results for 3 of 4 treatments).

The magnitude of runoff was very well predicted over the 5 year study for all but the CDS-NCC-MS treatment, however, the statistics for simulating runoff events were "poor". Unlike default DNDC or RZWQM, the NSE was ≥ 0 for revised DNDC for all validation treatments, however, the d statistic was low. Interestingly the statistics for cumulative runoff, often being the only statistics provided by some studies (Guest et al., 2018), were "good" to "excellent", with d ≥ 0.82 for both revised DNDC and RZWQM2 across all treatments. RZWQM2 overestimated runoff in the CDS-CC-MS treatment (Fig. 4.6), however as mentioned previously, the hydraulic parameters employed in the Brooks-Corey soil-water retention model are very sensitive. Below 20 cm depth these parameters were estimated using an internal curve fitting routine rather than being supplied from measured data. Note that total runoff + tile drainage were simulated with "good" model performance by RZWQM2 and "excellent" performance by revised DNDC across all treatments.

Similar to the Gilmore City location, the simulation of nitrogen loss to tiles by revised DNDC was improved over default DNDC at Woodslee and revised DNDC produced similar average statistics relative to RZWQM across the two CDS treatments with "fair" model performance (Table 4.6). Both models over-predicted N loss during the early stages of the study, then predicted less loss during 2002, with similar losses for the remainder of the study (Fig. 4.6). N movement to tiles in DNDC was strongly correlated with water movement (Fig. 4.6 a, b) and overall the cumulative losses were well simulated (d ≥ 0.76). The timing of N loss to runoff was not well simulated by either model but the cumulative loss was simulated with "fair" to "excellent" performance. Revised DNDC predicted a large N runoff event on June 21, 2002 at the time of 66.4 mm of precipitation which was not observed nor predicted by RZWQM2. It is likely that DNDC under-predicted the rate of N movement down the profile with too much N remaining in the top 2 layers (~3 cm depth). Note that default DNDC predicted nearly zero N in runoff as the fraction of N lost to runoff was set internally at a very low value and was only based on the top soil layer.

Revised DNDC simulated the appropriate reduction in N losses to tiles under controlled drainage relative to unrestricted drainage (Fig. 4.6, Table 4.S4). The reduction in N loss to drains from CDS for the CC treatments was -39.1%, -40.8% and -24.3% for observed, revised DNDC and RZWQM2, respectively (Fig. 4.6, Table 4.S4), whereas CDS reduced nitrate loss by -37.5%, -39.1%, and -20.2% for the NCC treatments compared to unrestricted tile drainage (Table 4.S4). Reduced N loss to tiles for controlled drainage relative to unrestricted drainage is a common finding in many studies (Drury et al., 2009, 2014b; Tan et al., 1993, 2007). Since soil N is a crucial driver for several biogeochemical processes, the successful simulation by revised DNDC expands the models accuracy and capabilities.

Table 4.6 Statistical performance of models for simulating water and N loss to runoff and tile drains at the Woodslee research site (n=28 over 5 years)

		--------- Calibration ---------			---------- Validation ----------								
		TD-CC-MS*			TD-NCC-MS			CDS-CC-MS			CDS-NCC-MS		
Water/N component	Statistic	Default DNDC	Revised DNDC	RZWQM	Default DNDC	Revised DNDC	RZWQM	Default DNDC	Revised DNDC	RZWQM	Default DNDC	Revised DNDC	RZWQM
Tile drainage	NARE	-5.8	-0.5	-5.3	7.0	11.7	1.3	NA	5.3	-7.9	NA	59.1	25.6
	NSE	0.08	0.88	0.59	-0.06	0.85	0.59	NA	0.75	0.64	NA	0.05	0.35
	d	0.67	0.96	0.88	0.68	0.96	0.89	NA	0.94	0.89	NA	0.83	0.82
Runoff	NARE	1.5	11.3	18.9	-10.2	-5.1	0.1	NA	-0.06	57.1	NA	-26.4	12.2
	NSE	-1.85	-0.18	-0.58	-0.58	0.13	-0.26	NA	0.11	-1.62	NA	0.16	-0.37
	d	0.65	0.66	0.62	-0.71	0.64	0.55	NA	0.68	0.60	NA	0.60	0.63
Runoff + tile drainage	NARE	-4.1	1.3	0.4	2.1	6.9	1.0	NA	3.6	10.3	NA	22.7	19.9
	NSE	0.53	0.90	0.48	0.48	0.89	0.40	NA	0.90	0.39	NA	0.77	0.14
	d	0.84	0.97	0.86	0.84	0.97	0.85	NA	0.97	0.86	NA	0.95	0.82
N loss to tiles	NARE	0.9	1.2	-4.4	-1.0	14.0	4.4	NA	-1.7	18.9	NA	11.0	33.0
	NSE	0.51	0.57	0.21	0.52	0.60	0.01	NA	0.46	0.56	NA	0.20	-0.30
	d	0.79	0.82	0.70	0.81	0.88	0.77	NA	0.78	0.84	NA	0.76	0.68
N to runoff	NARE	-97.7	-5.4	-29.0	-98.0	-23.6	-42.9	NA	-13.8	-27.8	NA	-2.6	-19.6
	NSE	-0.53	-3.57	0.02	-0.77	-3.83	-0.23	NA	-3.2	-0.48	NA	-5.15	-1.20
	d	0.39	0.51	0.57	0.41	0.45	0.52	NA	0.51	0.50	NA	0.47	0.34
N to runoff + tile drains	NARE	-12.4	0.3	-7.8	-15.0	8.6	-2.5	NA	-4.8	6.8	NA	8.2	22.0
	NSE	0.49	0.55	0.21	0.50	0.66	0.06	NA	0.29	0.54	NA	0.24	-0.20
	d	0.77	0.81	0.70	0.79	0.89	0.76	NA	0.70	0.82	NA	0.76	0.69

* TD – unrestricted tile drainage; CDS – controlled drainage and subsurface irrigation; CC – cover crop; NCC – No cover crop; MS - Maize-soybean rotation phase; SM – Soybean-maize rotation phase

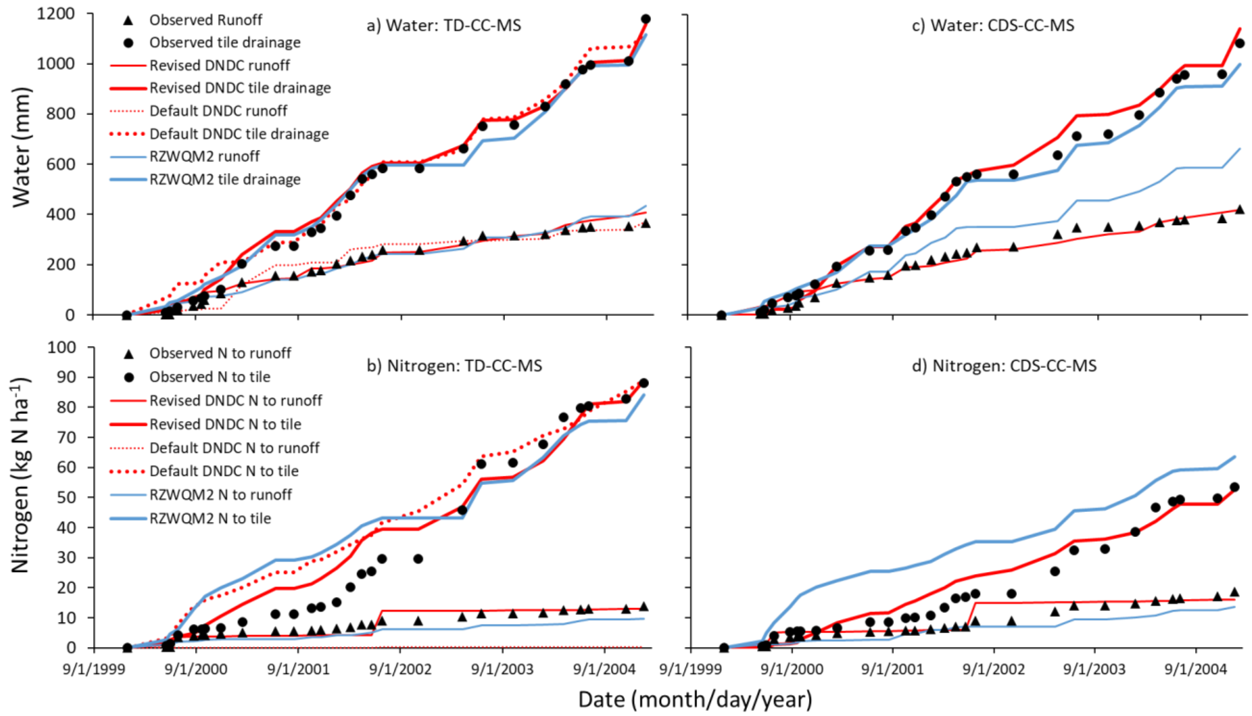

Figure 4.6 Observed and simulated cumulative water and N losses to runoff and tile drains at the Woodslee research site for a) water losses using unrestricted tile drainage, b) nitrogen losses using unrestricted tile drainage, c) water losses using controlled drainage with sub-irrigation and d) nitrogen losses using controlled drainage with sub-irrigation.

4.4 Conclusions

Inaccuracies in the simulation of water and N dynamics in the DNDC model have strongly impacted and impeded the further development of several related biogeochemical processes, particularly in the case of trace gas emission estimates. Prior to the developments implemented in this study, DNDC (Canada & U.S. versions) only simulated cascade water flux vertically down the soil profile without a mechanistic tile drainage algorithm. We implemented a deeper and heterogeneous soil profile, root penetration and density functions, a fluctuating water table, unsaturated flow above field capacity, and the Hooghoudt equation to simulate mechanistic tile drainage based on drain spacing, depth and tile diameter. After development, simulations of soil water storage, daily drainage, N loss to runoff and N loss to tile drains were improved, comparing well to measurements at two research sites and showing at least as good of performance as RZWQM2. This demonstrated that DNDC development was successful considering RZWQM2 is a well-validated water quality model which includes detailed computational hydrology. The soil-water input requirements for DNDC were kept relatively low and the model simulation time remains 4 times faster than RZWQM2. Model computation time is becoming less important in some regions of the world, however, the DNDC model has a wide array of users which sometimes still do not have easy access to supercomputers or related computation capacities. Likewise, readily available and easily understandable model inputs can expand the use of a model. The revised DNDC model did not simulate the timing of water or N losses to runoff well but performed satisfactory in simulating the cumulative magnitudes. The simulation of runoff is complex particularly when surface crusting, clay cracking, preferential flow through insect and root channels, snow dynamics, and soil freeze-thaw are prevalent and further research is recommended. Through these developments we have expanded the ability of DNDC to simulate the impacts of tile drainage management on several biogeochemical processes. Future studies can now investigate optimum tile drain depth and spacing, and explore possible benefits of controlled drainage or sub-irrigation.

4.5 Supplementary Tables and Figures

Table 4.S1 Measured soil physical and hydraulic properties at the Gilmore City (adapted from Qi et al., 2011b) and Woodslee sites

Depth (cm)	Sand (%)	Clay (%)	BD (g cm^{-3})	SOM (%)	K_{sat} (cm h^{-1})	Porosity	Θ_{10} (cm^3 cm^{-3})	Θ_{33} (cm^3 cm^{-3})	Θ_{1500} (cm^3 cm^{-3})
Gilmore City									
0-10	0.32	0.32	1.37	4.3	4.8*	0.482	0.383	0.376	0.189
10-20	0.32	0.32	1.38	3.8	3.3	0.476	0.384	0.376	0.230
20-30	0.33	0.14	1.39	3.3	5.1	0.473	0.384	0.376	0.201
30-40	0.4	0.30	1.39	1.3	4.1	0.474	0.384	0.399	0.212
40-60	0.46	0.24	1.39	1.3	4.1	0.474	0.408	0.368	0.218
60-90	0.44	0.20	1.45	0.6	2.6	0.450	0.380	0.368	0.204
90-120	0.44	0.20	1.46	0.5	2.6	0.450	0.312	0.299	0.184
120-200	0.44	0.20	1.46	0.5	0.01	0.450	0.310	0.299	0.168
Woodslee									
0-10	0.28	0.37	1.39	2.6	1.15*	0.474	0.374	0.338	0.243
10-20	0.28	0.37	1.45	2.4	1.05	0.453	0.376	0.346	0.256
20-60	0.28	0.37	1.45	0.9	0.95	0.453	0.376	0.346	0.256
60-100	0.28	0.37	1.45	0.3	0.91	0.453	0.376	0.346	0.256
100-150	0.28	0.37	1.45	0.1	0.91	0.453	0.376	0.346	0.256
150-200	0.28	0.37	1.45	0.1	0.01	0.453	0.376	0.346	0.256

BD = bulk density; SOM = soil organic matter; K_{sat} = saturated hydraulic conductivity; θ_{10}, $\theta_{33,}$ θ_{1500} = soil water content at pressure 10, 33 and 1500 Kpa, respectively

* K_{SAT} was calibrated

Table 4.S2 Model parameters used in the default and revised DNDC model for Gilmore City and Woodslee research sites

Sites	**Gilmour City**						**Woodslee**					
	Default DNDC			Revised DNDC			Default DNDC			Revised DNDC		
Crop Parameters	Maize	Soybean	Winter Rye	Maize	Soybean	Winter rye	Maize	Soybean	Winter wheat	Maize	Soybean	Winter wheat
Max grain (kg C ha^{-1} y^{-1})	4500	2550	900	4500	2400	900	4900	1950	2500	4600	1800	2500
Grain fraction	0.4	0.35	0.28	0.4	0.35	0.28	0.45	0.30	0.41	0.45	0.34	0.41
Stem+leaf fraction	0.44	0.44	0.46	0.44	0.44	0.46	0.43	0.44	0.42	0.43	0.44	0.42
Root fraction	0.16	0.21	0.25	0.16	0.20	0.25	0.12	0.26	0.17	0.12	0.22	0.17
Grain C:N	35	10	20	35	10	20	35	10	35	30	10	35
Stem+leaf C:N	70	30	50	70	35	50	70	30	85	50	30	85
Root C:N	70	15	50	70	20	50	70	15	85	60	15	85
Water demand (gH_2O gDM^{-1})	135	420	150	120	340	150	136	420	150	110	300	150
GDD (0^oC base)	2550	2500	1400	2650	2650	1400	2200	2200	1400	2300	2300	1400
Optimum temperature (^oC)	30	25	18	30	25	18	30	25	14	30	25	14
Max root depth (m)	NA	NA	NA	1.35	1.35	1.5	NA	NA	NA	0.8	1.1	NA
Initial Soil Parameters												
Litter fraction		0.01			0.01			0.01			0.01	
Humads fraction		0.29			0.09			0.24			0.082	
Humus fraction		0.70			0.90			0.75			0.908	
Humads C:N ratio		10			10			11			11	
Humus C:N ratio		10			10			11			11	
Runoff and Tile Drainage												
Tile spacing (m)		NA			7.6			NA			7.5	
Drain radius (m)		NA			0.0768			NA			0.1	
Tile depth (m)		NA			1.06			NA			0.65	
Preferential N movement		NA			2%			NA			2%	
Runoff curve number		64			64			87			87	
Manning's coefficient		0.19			0.19			0.19			0.19	

Table 4.S3 Calibrated crop parameters used in RZWQM2 for corn, soybean and winter rye at the Gilmore City and Woodslee locations (Gilmore City adapted from Smith et al., 2019c)

Crop	Parameter	Parameter description	Glimour City	Woodslee
Corn[a]	G2	Maximum possible number of kernels per plant	722	650
	G3	Kernel filling rate during linear grain filling stage under optimum conditions (mg d^{-1})	6.55	6.0
	PHINT	Phyllochron interval between successive leaf tip appearance	46	48
Soybean[b]	LFMAX	Max leaf photosynthesis rate (μmol CO_2 m^{-2} s^{-1})	0.8	0.63
	SLAVR	Specific leaf area of cultivar under standard growth conditions (cm^2 g^{-1})		280
	SIZLF	Maximum size of full leaf (three leaflets) (cm^2)		122
	XFRT	Maximum fraction of daily growth that is that is portioned to seed + shell		0.77
	WTPSD	Maximum weight per seed (g)		0.17
Winter rye[c]	PEG	Germination phase duration (ºC d cm cm^{-1})	75	
	PECM	Emergence phase duration (ºC d cm cm^{-1})	25	
	P1V	Relative amount that development is slowed for each day of unfulfilled vernalization, assuming 50 d is sufficient	5	
	P1D	Relative amount that development is slowed when plants are grown in photoperiod 1 hour shorter than optimum (d)	12	
	PARUV	Conversion rate for photosynthetically active radiation to dry matter before the end of leaf growth (g MJ^{-1})	3.3	
	LAVS	Area of standard vegetative stage leaf (cm^2)	15	
	LARS	Area of standard reproductive phase leaf (cm^2)	25	
	LARWS	Lamina area to weight ratio of standard first leaf (cm^2 g^{-1})	300	
	LAWR2	Lamina area to weight ratio, phase 2 (cm^2 g^{-1})	280	
	P5	Relative grain filling duration based on thermal time (d)	400	
	PHINT	Phyllochron interval between successive leaf appearance (PD)	100	

[a] Cultivar IB1 068 Dekalb 521
[b] Cultivar 990002 M Group 2
[c] Cultivar 990003 Winter-US, Winter wheat crop parameters were adjusted to simulate winter rye at Gilmore City site, but default parameters were used for the winter wheat grown at Woodslee

Table 4.S4 Observed and simulated total water and N loss to runoff and tiles at the Woodslee site from winter of 1999 to early 2005

Treatment	RUNOFF				DRAINAGE				RUNOFF + DRAINAGE			
	Observed	Default DNDC	Revised DNDC	RZWQM	Observed	Default DNDC	Revised DNDC	RZWQM2	Observed	Default DNDC	Revised DNDC	RZWQM2
					Water losses (mm)							
TD-CC-MS	365	371	407	434	1179	1111	1158	1116	1545	1482	1565	1551
TD-NCC-MS	438	393	415	438	1097	1173	1225	1111	1535	1567	1641	1550
CDS-CC-MS	422	NA	420	663	1086	NA	1143	1000	1508	NA	1563	1664
CDS-NCC-MS	590	NA	434	662	795	NA	1265	999	1386	NA	1700	1661
					Nitrogen losses (kg N ha^{-1})							
TD-CC-MS	13.8	0.3	13.1	9.8	88	88.8	89.1	84.1	101.8	89.2	102.1	93.9
TD-NCC-MS	17.2	0.3	13.2	9.8	102	100.9	116.3	106.4	119.2	101.1	129.5	116.3
CDS-CC-MS	18.8	NA	16.2	13.5	53.6	NA	52.7	63.7	72.3	NA	68.8	77.2
CDS-NCC-MS	16.9	NA	16.4	13.6	63.7	NA	70.8	84.8	80.6	NA	87.2	98.3

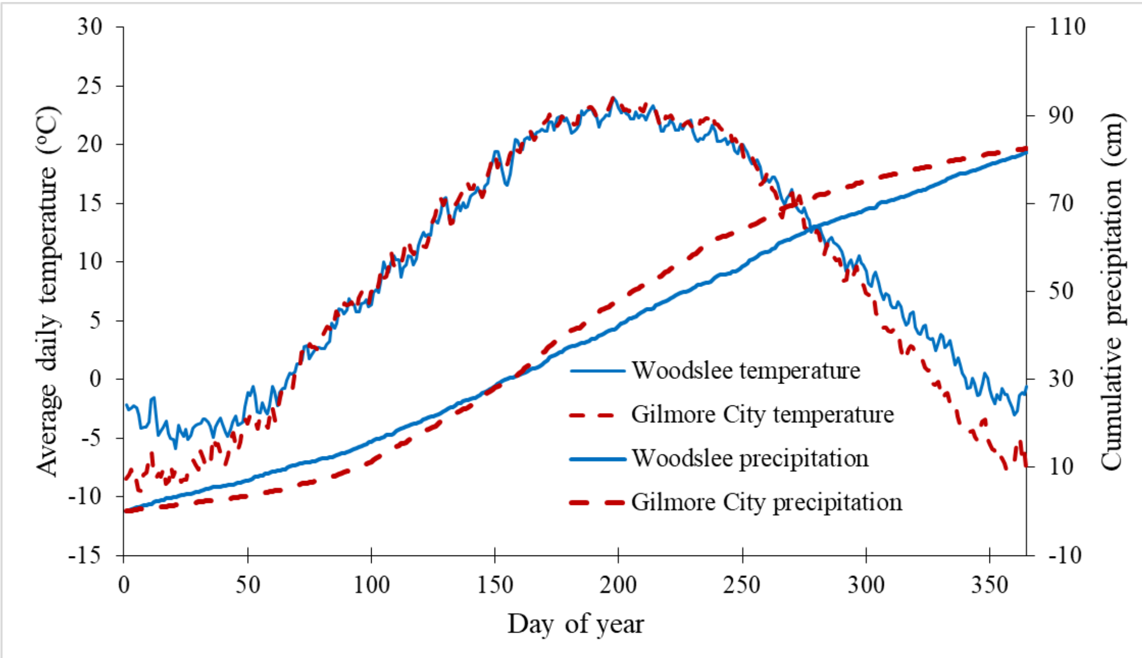

Figure 4.S1 Average temperature and precipitation at the Gilmore City and Woodslee sites.

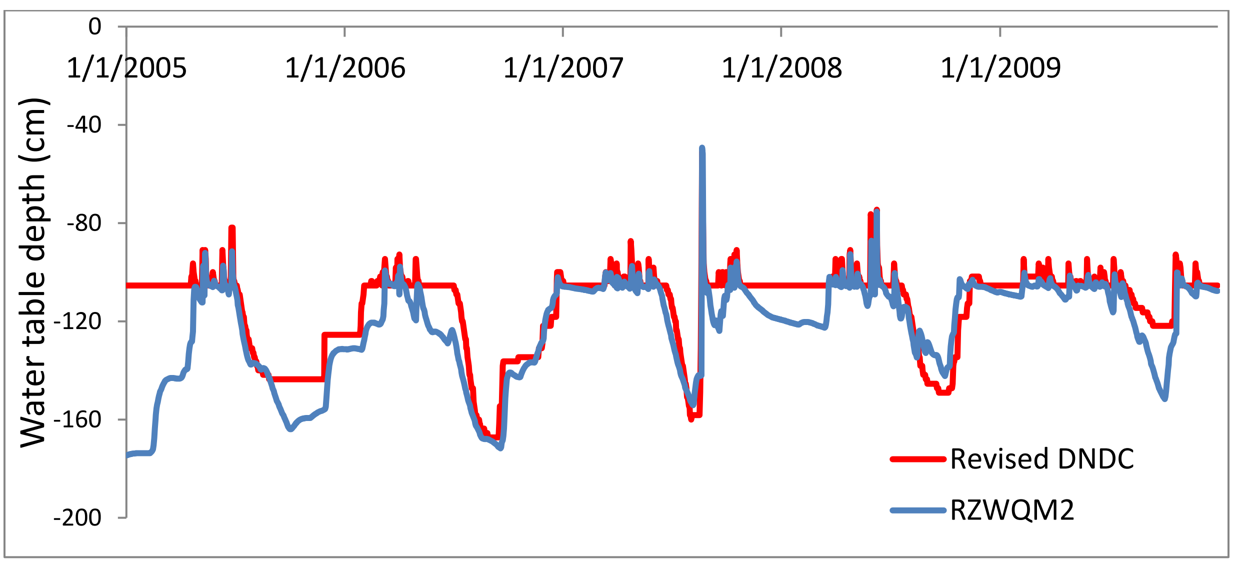

Figure 4.S2 Simulation of water table depth below the soil surface for a maize-soybean rotation with cover crop at Gilmore City research site in Iowa

Connecting text to Chapter 5

In Chapter 4 several developments were implemented in DNDC which improved its performance for simulating soil hydrology and N losses to tile drains. The inclusion of the drainage sub-model was of particular importance since it allowed for the consideration of drainage design impacts on water and nutrient cycling, extending the functionality of the model. After developments, the DNDC model could be used as a more accurate and comprehensive tool for assessing trade-offs in reactive N losses (NO_3^- loss to drains and runoff, N_2O emissions, NH_3 volatilization) which was a primary purpose for the research. In Chapter 5 the revised model was employed to explore reactive N losses for 18 fertilizer management sceneries across 30 years of climate variability at locations in eastern Ontario and the US Midwest. A wide range of fertilizer management recommendations were made and the trade-offs in losses were documented. Simulations were performed at the two locations where the model was evaluated in Chapter 4 but also at a location near Ottawa, Ontario (Alfred) where a colleague, in cooperation with Ward Smith and Dr. Zhiming Qi, successfully evaluated the revised model for simulating N_2O emissions, drainage, and N losses to tile drains (He et al., 2019b).

The following manuscript was published in the Journal of Environmental Quality:
Smith, W., B. Grant, Z. Qi, W. He, A. VanderZaag, C.F. Drury, X. Verge, H. Balde, R. Gordon, and M. Helmers. 2019. Assessing the impacts of climate variability on fertilizer management decisions for reducing nitrogen losses from corn silage production. Journal of Environmental Quality. 48(4):1006-1015. doi:10.2134/jeq2018.12.0433

Chapter 5

Assessing the impacts of climate variability on fertilizer management decisions for reducing nitrogen losses from corn silage production

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Abstract

There is an incentive for dairy farmers to maximize crop production while minimizing costs and environmental impacts. In cold climates, farmers have limited opportunity to balance field activities and manure storage requirements while limiting nutrient losses. A revised DeNitrification DeComposition (DNDC) model for simulating tile drainage was used to investigate fertilizer scenarios when applying dairy slurry or urea on silage corn (Zea mays L.) to examine N losses over a multidecadal horizon at locations in eastern Canada and the US Midwest. Management scenarios included timing (spring, fall, split, and sidedress) and method of application (injected [10 cm], incorporated [5 cm], and broadcast). Reactive N losses (NO_3^- from drainage and runoff, N_2O, and NH_3) were 2.6, 1.8 and 3.0 times greater per metric ton of silage biomass from the sandy loam soils than from the finer textured clay or clay loam soils at Alfred, Woodslee and Gilmore City, respectively. Regarding fertilizer placement, N losses were greatest from broadcast, followed by incorporated and then injected applications. Among the fertilizer timing scenarios, fall manure application resulted in the greatest N loss, primarily due to increased N leaching in non-growing-season periods, with 58% more N loss per metric ton of silage than spring application. Split and sidedress mineral fertilizer had the lowest N losses, with average reductions of 9.5 and 4.9%, respectively, relative to a single application. Split application mitigated losses more so than sidedress by reducing the soil pH shift due to urea hydrolysis and NH_3 volatilization during the warmer June period. This assessment helps to distinguish which fertilizer practices are more effective in reducing N loss over a long-term time horizon. Reactive N loss is ranked across 18 fertilizer management practices, which could assist farmers in weighing the tradeoffs between field trafficability, manure storage capacity, and expected N loss.

5.1 Introduction

Dairy farming is one of the largest agricultural sectors within the cooler climatic zones of eastern Canada (AAFC, 2017) and the US Midwest (USDA, 2018). It is important that opportunities be identified for managing on-farm nutrient cycling in an efficient and cost effective manner (Holly et al., 2018). Using base calculations from Sheppard and Bittman (2016) the total combined N losses from cropping systems in Canada represent ~27% of the value of fertilizer shipped to farms. A much larger cost could be expected in response to environmental damage and harm to human health. In order to establish beneficial management practices (BMPs) a sound understanding of the impacts on nutrient losses is required. In cold climates, snow dynamics, freeze-thaw actions and stresses on crops complicate the biophysical processes which need to be considered when accessing nutrient loss. As well, farmers must manage their field operations with consideration of a shorter growing season along with manure storage implications.

Field studies are critical for assessing impacts of management on reactive N loss, however, they are limited in their ability to simultaneously characterize multiple N loss pathways and long-term impacts of climate variability. Process based models are well suited for assessing management impacts in cropping systems (Brilli et al., 2017; Ma et al., 2007a; DeJong et al., 2009) since they can dynamically simulate many of the interdependent soil-plant-atmospheric processes over space and time. A well calibrated model can be employed to simulate the long-term impacts of climate variability and management on N losses from cropping systems (Congreves et al., 2016a; Qi et al., 2011b).

Although many agricultural models were originally developed to simulate a single output such as crop growth, soil carbon change, water quality, or greenhouse gas emissions, there has been increased effort to enhance models to include a larger scope of agricultural processes (Ma et al., 2007). Three models are predominantly used in the cooler regions of North America, as they all characterize overwinter snow dynamics and soil freeze–thaw events. The DeNitrification DeComposition model (DNDC; Li et al., 1992) was originally developed to estimate N_2O emissions, whereas DayCent (Parton et al., 2001) focused more on soil C, and the Root Zone Water

Quality Model (RZWQM2; Flerchinger et al., 2000; Ma et al., 2012) focused on water quality and crop growth. However all three models have been expanded to simulate all four outcomes.

A Canadian version of the DNDC model was developed to improve the simulation of crop growth, snow dynamics, NH_3 volatilization, impacts of winterkill, and mechanistic tile drainage in cool weather conditions (Kroebel et al., 2011; Smith et al., 2013; Congreves et al., 2016b; Dutta et al., 2016a, 2016b, 2018; Jarecki et al., 2018). The model has been validated for simulating N_2O emissions (Uzoma et al., 2015; Abalos et al., 2016; Congreves et al., 2016a; He et al., 2018) and NH_3 volatilization (Congreves et al., 2016b; Dutta et al., 2016a) for numerous cool climate locations. It has been applied by Abalos et al. (2016) to examine the effectiveness of various types of 4R fertilizer management (right source, right rate, right time, and right place) toward reducing N_2O emissions from corn (Zea mays L.) production in eastern Canada. Congreves et al. (2016a) expanded on this concept to examine the impacts of climate variability on reactive N loss in a conventional and best management cropping system at a site in eastern Ontario. There has, however, been limited effort to date in investigating fertilizer management that may reduce overall reactive N loss from cropping systems relevant to dairy production, particularly in considering the resiliency under climate variability. Furthermore, recent model developments now allow for the estimation of N loading to tile drains.

The objectives of this study were (i) to use the revised DNDC model to investigate inorganic and organic fertilizer management practices over a 30-yr time horizon to determine practices that may reduce reactive N loss from corn silage production in cool climatic zones of eastern Canada and the US Midwest, and (ii) to examine tradeoffs and synergies between N loss to tile drains, N loss to runoff, NH_3 volatilization, and N_2O emissions and recommend beneficial management.

5.2 Materials and methods

Climate and soils data from the experimental sites at Alfred, Ontario; Woodslee, Ontario and Gilmore City, Iowa were used to explore the impacts of 18 fertilizer management scenarios with the DNDC model. A general description of the sites are included in supplementary material (Supplemental Section 5.S1, table 5.S1) but note that the corn silage cultivar and farming practices employed in our modelling assessment were the same for each site. These were based on management at Alfred, the only site where a field experiment was conducted with corn silage.

5.2.1 DNDCv.CAN model: Description and Development

The DNDC model is a well-known process-based model (Li et al., 1992, 2012) for simulating trace gas emissions and C&N cycling in agri-ecosystems. The model framework is composed of four major components characterizing crop growth, soil temperature and water dynamics, denitrification and nitrification pathways and decomposition. A core strength of the modelling framework is in its ability to characterize a wide array of crop management activities while enforcing a mass balance of nutrient and water budgets. Pertinent N model outputs to this study include daily N losses to tile flow and leaching, runoff, trace gas emissions, and crop N uptake. A brief description of these processes are provided in Supplemental Section 5.S2.

Over the past seven years, the Canadian version of DNDC (DNDCv.CAN) was developed, first to include improved crop growth (Kroebel et al., 2011; Smith et al., 2013) including temperature stresses for cultivars grown in Canada (Yan and Hunt., 1999). More recently, alfalfa (*Medicago sativa* L.) growth was improved and a winter kill sub-model was incorporated (He et al., 2019a). Additionally, the simulation of evapotranspiration (Dutta et al., 2016b) and the impact of snow dynamics, crop biomass and residue management on soil temperature were improved (Dutta et al., 2018). In cool climates more than half of annual N_2O emissions may be related to freeze-thaw processes (Wagner-Riddle et al., 2017). The DNDC model previously did not include textural dependent soil heat transfer and had a very simple approximation of snow insulation. The inclusion of these processes improved the simulation of soil temperature resulting in an improved model for estimating N_2O emissions after thaw events (Dutta et al., 2018). Furthermore, a new NH_3 volatilization sub-model was included for manures (Congreves et al., 2016b) and urea (Dutta et al., 2016a) using cool climate datasets from Quebec. A model inter-comparison demonstrated that DNDCv.CAN performed as well as the computationally intensive RZWQM2 for simulating crop biomass, and monthly water flow and N loss to tile drains but daily simulation of drainage and soil water storage was not as well simulated (Smith et al., 2019c). Based on these findings we developed DNDCv.CAN to include both a heterogeneous and deeper soil profile (2m), root penetration and density functions, improved water flow, a fluctuating water table, and mechanistic tile drainage (Smith, unpublished data , 2019). The model version used in this study is available for download at (https://github.com/BrianBGrant/DNDCv.CAN).

5.2.2 Model Calibration and Validation at Experimental Sites

The DNDCv.CAN model has undergone extensive improvement and validation for simulating losses of reactive N from agriculture in cool climates. In this study we leverage previous developments for simulating N_2O emissions (He et al., 2018a; Uzoma et al., 2015) and NH_3 volatilization (Dutta et al., 2016a Congreves et al., 2016b), which remain unchanged in the model. We also summarize the performance of the model for i) simulating drainage and N loss to drains using the more recently incorporated mechanistic drainage algorithms at Alfred, Woodslee and Gilmore City (Supplemental Section 5.S3; Tables 5.S2, 5.S3) and ii) simulating corn silage biomass, corn silage N uptake, N_2O emissions, and soil NO_3^- at the Alfred site (Supplemental Section 5.S4, Table 5.S4). We used the model parameterization from this previous work in our modelling assessment, simulating the same silage cultivar (Table 5.S5) and management practices across the three locations. The soils and drainage parameterization for the fine textured soils was employed at each respective location. This data was, however, not available for coarser textured soils thus we derived appropriate properties and drainage characteristics for a sandy loam and used these across all three locations (Table 5.S5). The soil hydraulic properties for the sandy loam were determined using the pedotransfer functions in the Soil–Plant–Atmosphere–Water model (SPAW) (Saxton and Willey, 2006). Since the sandy loam was of higher permeability we set the tile drain depth to 1.4 m and spacing to 30 m, which is the minimum recommended spacing for this soil type (ASAE, 2015). Although the inclusion of a sandy loam texture allows us to explore N losses that may occur from a high permeability soil the model has not been validated for this soil type thus we expect higher uncertainty in results.

5.2.3 Modelling approach for simulating climate variability and management impacts on N losses

The DNDC model was used to explore 18 fertilizer management scenarios (Table 5.1) across 30 years of climate variability at the three locations for their impacts and trade-offs on N_2O emissions, NH_3 volatilization, N leaching and runoff. Two soil textures were simulated at each location, a fine textured soil for which the model was previously validated for simulating water and N losses and a sandy loam texture (see section 5.2.2 for soil and drainage characteristics). To represent a cropping system used by dairy farmers we simulated a 5-year alfalfa-alfalfa-alfalfa-corn silage-corn silage rotation, repeating 3 times over 15 years. Climate data was interchanged according to the flowchart (Fig. 5.1) with each of the 30 years of weather being simulated for each of the 18 fertilizer scenarios, whereby each specific weather year covered a two year period to ensure that we compared the same weather year in the fall to fall or spring to spring simulations. The results were analysed either from the timing of fall to fall or from spring to spring fertilizer application thus the same total annual precipitation was applied for each year of analysis. A 16th year was simulated to assess N loss from spring to spring fertilizer application.

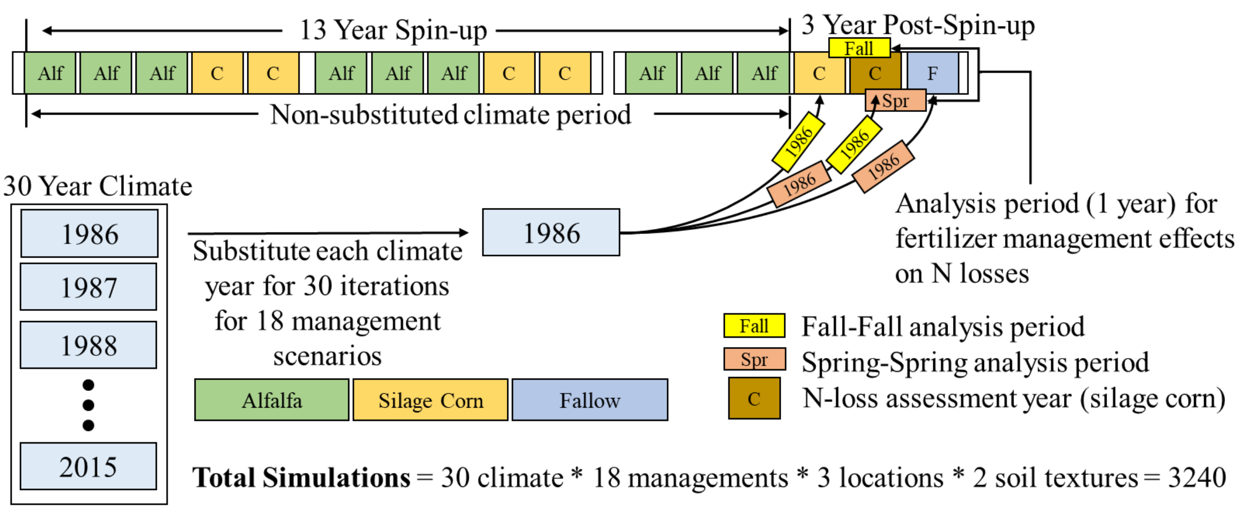

Figure 5.1. Schematic of climate substitution approach for investigating climate variability impacts on fertilizer management

To assess climate variability, a 30-yr climate normal (1986–2015) was constructed from a combination of onsite multi-environment trial data collected at each location and climate data obtained from the Nasa Prediction of Worldwide Energy Resources (POWER) Project datasets (https://power.larc.nasa.gov/). It is important to emphasize that each one of the climate years from the 30 year climate normal was simulated independently for each fertilizer management to quantify each year of climate variability. This was coupled to a standardized 13-year spin-up simulation to stabilize C, N, and water cycling that remained consistent across all fertilizer management scenarios.

The fertilizer scenarios consisted of 3 methods of application (surface broadcast, broadcast and incorporated to 5cm, and injected to 10cm). For each method of application the following fertilizer scenario was employed; spring mineral fertilizer (urea), spring mineral side-dress (urea), spring mineral split (urea), spring organic (manure-slurry), spring split organic (manure-slurry), and fall organic (manure-slurry) (Table 5.1). The fertilizer rate on corn silage was set to 100 kg N ha^{-1} for the first year after alfalfa and 140 kg N ha^{-1} (rate used at local Alfred site) for the second year. In the broadcast scenarios an additional 40 kg N ha^{-1} was applied to account for higher NH_3 losses and ensure production levels remained reasonably consistent across treatments (Drury et al., 2017). The dairy manure slurry composition was based on the slurry applied at Alfred (He et al., 2019b). In this study we simulated soils which are well drained increasing the chance of field trafficability limiting excess crop water stress, and allowing for more consistent planting dates. For all simulations the silage corn planting date was set to May 10th, the spring and pre-plant fertilizer was applied on May 10th, the sidedress and split on June 8th, and tillage events were May 9th (disk plow) and October 30th (mouldboard plow). Fall manure was applied on November 1st.

The DNDC model inputs were constructed using R statistical software (R Core Team, 2013) to build the 3240 iterative permutations of climate and management and soil type. The N losses associated with each fertilizer practice were computed over a single annum, from spring to spring or fall to fall, depending on how the management was applied.

Table 5.1 Description of Fertilizer Management Scenarios employed across 3 study locations on a silage corn cropping system

Fertilizer Application Type	Spring Mineral	Spring Split Mineral	Spring SideDress Mineral	Spring Organic	Spring Split Organic	Fall Organic
Description	Applied at seeding	50% applied @ seeding 50% applied at V6 stage	Starter 30 kg ha^{-1} applied @ seeding 110 kg ha^{-1} applied at V6	Manure applied at seeding	50% of manure applied @ seeding: 50% at V6 stage	Manure Applied in Fall
Rate of N Applied* (kg N ha-1)	140	140	140	organic 108 inorganic 104#	organic 108 inorganic 104	organic 108 inorganic 104
Type of Fertilizer	Urea	Urea	Urea	Manure-Slurry	Manure-Slurry	Manure-Slurry
Fertilizer Acronym						
Injected (10cm)	iSM	iSpM	iSdM	iSO	iSpO	iFO
Incorporated (5cm)	ISM	ISpM	ISdM	ISO	ISpO	IFO
Broadcast	BSM	BSpM	BSdM	BSO	BSpO	BFO

* Broadcast N rates were +40 kg N ha^{-1} higher than other treatments for urea and manure slurry. For slurry, the organic and inorganic components were increased proportionately.
# inorganic component ~ 98% NH_4^+ and 2% NO_3^-

5.2.4 Statistical Analysis

Statistical analysis was conducted using one-way ANOVA in the SPSS 20.0 package (IBM Corp., 2011). Duncan's test at the 0.05 level ($p < 0.05$) was used to determine whether there are any statistically significant differences between treatments within the same soil texture.

5.3 Results and Discussion

The revised DNDC model, which includes the capacity to simulate mechanistic tile drainage, was successfully calibrated and validated using hydrology and N loss data from Alfred (He at al., 2019b), Woodslee and Gilmore City (Smith, unpublished data , 2019). The validation, as described in supplementary material (Supplemental Section 5.S3, Tables 5.S2, 5.S3), demonstrates that the model can accurately simulate drainage and N loading to tiles, which expands the model's ability to assess multiple interactions and trade-offs in reactive N losses. Our study is the first time the newly revised and validated model is used to examine multiple N loss pathways across multiple sites and the premise of this validation work was conceived in part to facilitate this study. The model also performed well in simulating crop corn silage biomass, crop N uptake for corn silage, soil N, and N_2O emissions at the Alfred location (Supplemental Section 5.S4, Table 5.S4).

5.3.1 Differences in climate between locations

The Alfred site has a considerably cooler climate than Woodslee or Gilmore City, lower wind speed, higher relative humidity (Fig. 5.S1, 5.S2) and thus lower evaporative losses. The annual average temperature at Woodslee is warmer than the Gilmore City site in Iowa with a similar growing season temperature but a warmer winter. As a consequence, winter snow cover is much greater at Alfred, followed by Gilmore City and then Woodslee. This influences both runoff and drainage volumes with, for instance, a larger amount of runoff occurring during spring snowmelt at Alfred. This helps emphasize the need for a model to be able to well characterize snow dynamics and soil freeze-thaw. Annual precipitation is greater at Alfred (1021 mm) and the overall annual magnitude is similar between Woodslee (816 mm) and Gilmore City (821 mm), but the seasonal trend is noticeably different (Fig. 5.S1). The Woodslee site has more over-winter precipitation and less growing season precipitation which results in more runoff at Woodslee, further supported by observations at Woodslee (Drury et al., 2014b) and water-balance simulations at Gilmore City (Qi et al., 2011b). In the DNDC model, N losses to runoff, drainage and N_2O emissions are strongly impacted by precipitation, which is the most variable weather driver at all three locations (Fig. 5.S2).

5.3.2 Understanding impacts of climate variability and fertilizer management on N losses from cropping systems

Variability in weather from year to year can make it difficult to determine the overall impact of management on N losses using field studies conducted over a short time horizon. In their assessment of combined BMPs for reducing N losses, Congreves et al. (2016a) found that management was more important than climate; however, climate variability can certainly be the more important factor, depending on which management is considered. In our study, we simulated the impacts of climate variability over 30 yr for 18 management scenarios across two soil types and at three locations. Our methodology allows for the direct assessment of climate impacts, since the cropping history was kept constant for each simulation.

Results were often highly variable across climate as is demonstrated in Figs. 5.2, S3 and S4. The results demonstrate the simulated variability associated with each site for harvestable silage biomass, N leaching to tiles, N_2O emissions, NH_3 volatilization and N loss to runoff, for 8 selected fertilizer managements. At Woodslee (Fig. 5.2), biomass, N leaching and N_2O emissions are generally highly variable across climate, both for the clay loam and sandy loam. Ammonia emissions are higher for the broadcast treatments and N runoff is notably higher only under fall applied manure, but again these are highly variable across the 30 years of climate. This is to be expected considering environmental drivers are known to have a strong impact on each of these outcomes (Congreves et al., 2016a; Holly et al., 2018). Across the three locations we see some common trends. For instance, N leaching, N runoff and N_2O emissions are higher and NH_3 volatilization is lower under fall applied manure than under spring applied manure. This is consistent with observations at Alfred (Schwager et al., 2016; Supplemental Section 5.S5). Broadcast fertilizer results in greater overall N losses. Biomass was ~23% lower in the sandy loam across the three locations due to both increased water and N stress. This is particularly true for Gilmore City and Woodslee which show more crop water stress, more-so at Woodslee which experiences more off-season runoff and has less growing season rainfall than at Gilmore City (Fig. 5.S1). Across the clay soils, the highest average and most variable N leaching occurred at Gilmore City. This high variability is consistent with site measurements where N loss to tiles under injected mineral fertilizer varied from 12.8 to 60.2 kg N $ha^{-1}y^{-1}$ across 5 years of measurements from corn (Smith et al., 2019c; Qi et al., 2011a, b). Our results from the 30 year simulations produced a range of 5.6 to 47.3 kg N $ha^{-1}y^{-1}$ under injected spring mineral fertilization on corn silage but 20 kg N ha^{-1} less fertilizer was applied in our study. The highest average N_2O emissions were simulated for the Woodslee clay loam versus the other sites, due to higher temperatures than at Alfred and lower soil permeability than at Gilmore City. Drury et al. (2014a) measured 7.36 kg N_2O-N $ha^{-1}y^{-1}$ from fertilized corn at Woodlsee and this is consistent with our average results for corn silage. As reported in many studies, these emissions are highly variable, as they are strongly affected by interannual variability of weather drivers (Uzoma et al., 2015; Smith et al., 2004) and they are usually higher from finer textured soils (Rochette et al., 2018).

Due to high variability it becomes difficult to discern difference among many fertilizer treatments, but these differences will be clarified using numerical and statistical methods in the following sections. Our results suggest that climate variability impacts may in some cases be greater than fertilizer management impacts and thus it could be challenging to discern differences when analysing only a few years of experimental measurements. Certainly though, experimental studies are essential for discerning shorter term impacts of weather events on processes which influence reactive N losses and trade-offs. This will lead toward having better characterized processes and algorithms which are crucial for developing improved models.

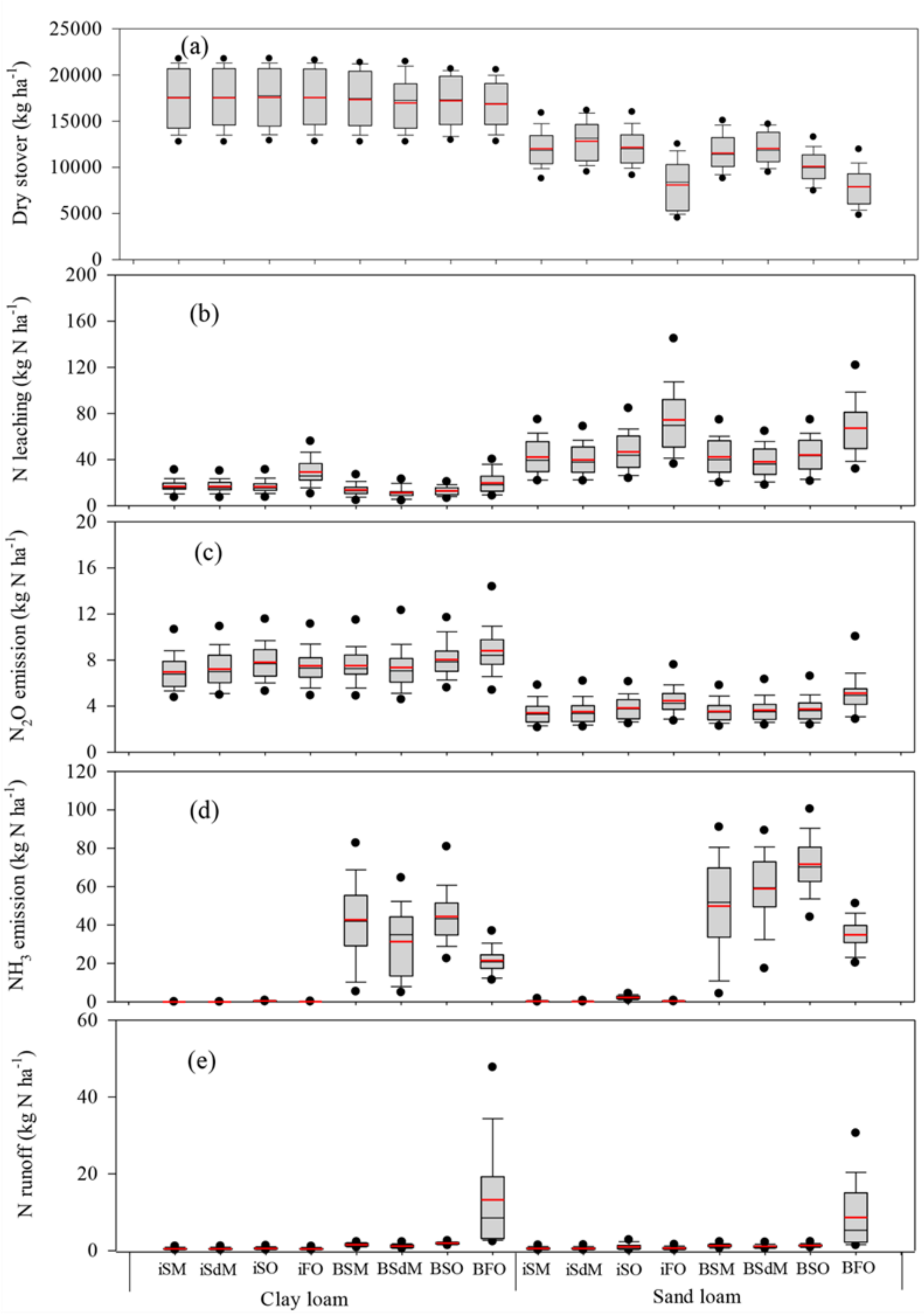

Figure 5.2. Boxplots showing simulated impacts of selected fertilizer management across 30 years of climate variability at the Woodslee location on a) dry silage biomass b) N leaching to tiles, c) N_2O emissions, d) NH_3 volatilization, and e) N runoff. The black and red lines, lower and upper edges of the boxes, and bars and dots in outside the boxes represent median and mean values, 25th and 75th, 5th and 95th, and <5th and >95th percentiles of all data, respectively.

5.3.3 Management impacts which are commonly studied experimentally

5.3.3.1 Fall versus spring applied organic fertilizer

To further demonstrate the variability that can occur across 30 years of climate, an example model output which highlights the differences over the time series in simulated N_2O emissions, NO_3^- leaching and NH_3 volatilization between spring and fall applied manure slurry is shown in Fig. 5.3. For this example using a clay soil at Alfred, the DNDC model predicted greater average N_2O emissions, N leaching and N runoff but less NH_3 volatilization in the fall than in the spring. This result was consistent across locations (Fig. 5.S5). The greater N_2O emission from fall applied manure were primarily caused by more substrates (i.e. soil N and dissolved organic C (DOC)) being available during the off-season freeze-thaw period, which enhances denitrification in DNDC. This is consistent with observations for the raw manure at Alfred (He et al., 2019b; Schwager et al., 2016). Thorman et al. (2008) found greater N_2O emissions when slurry was applied in late fall or winter than when applied in the spring. Non-growing season periods, when plant N uptake does not occur, are often favourable for denitrification (Rochette et al., 2004; Wagner-Riddle et al. 2008). Greater N leaching and runoff losses are generally expected from fall applied organic or inorganic fertilizer when soil moisture is high and due to losses during snow melt and freeze-thaw dynamics (Gamble et al., 2018; Schwager et al., 2015, 2016; Drury et al., 2016; Thorman et al., 2008; van Es et al., 2006; Randall et al., 2003; Di et al., 1999). Ammonia volatilization is lower simply due to lower average temperatures in the fall. For injected (Fig. 5.3a) and incorporated (Fig. 5.3b) scenarios, average N_2O emissions are less under spring than under fall applied slurry but in certain years more emissions occur under spring application depending on weather conditions. For instance, rainfall was exceptionally low in the 4 week period after slurry application in the fall of 1993 (66% of normal) resulting in lower than average N_2O emissions whereas an average level of rainfall in 1993 after spring slurry application resulted in a moderate level of emissions. Nitrogen loss due to leaching was generally higher for fall-applied manure than for spring-applied manure, but this was not always the case. This demonstrates the importance of taking measurements over a long timeframe or using well-validated models to extrapolate across climate variability.

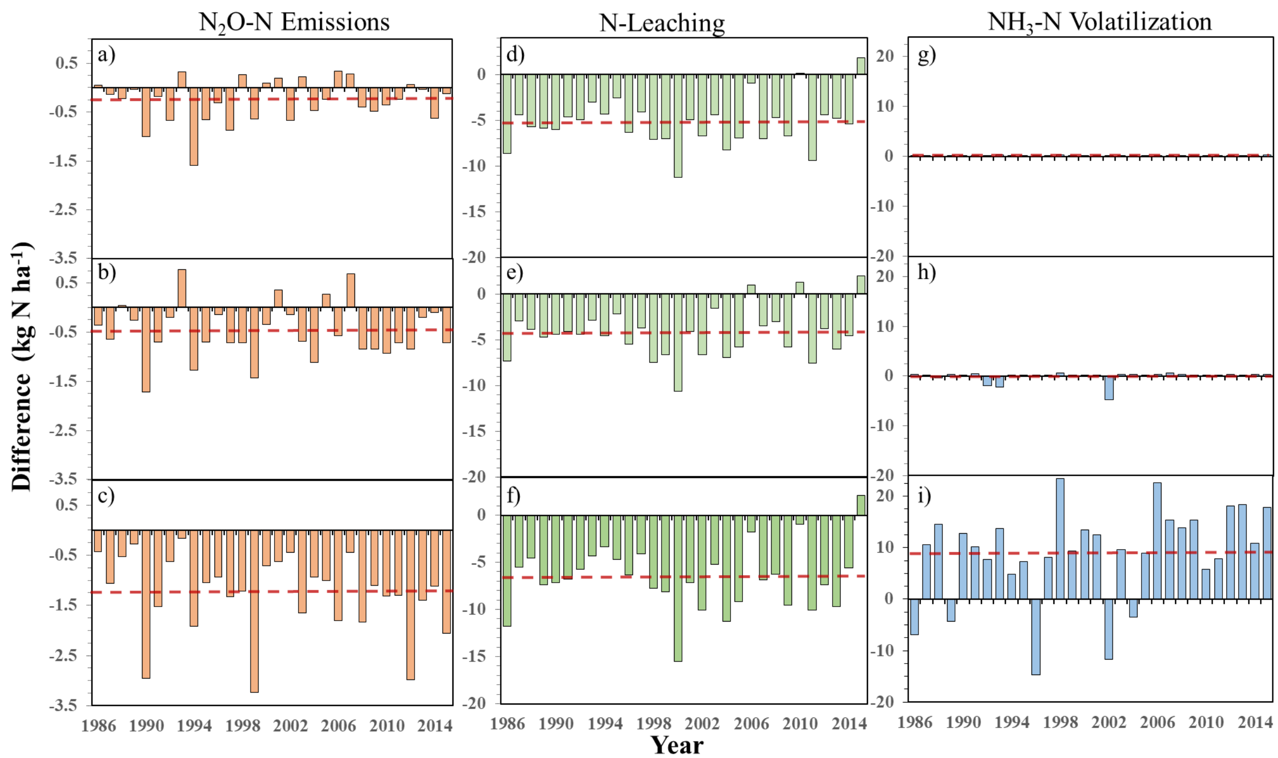

Figure 5.3. Differences in simulated reactive N loss between spring and fall applied manure (spring minus fall) for the clay soil at Alfred for N_2O emissions a) iSO-iFO, b) ISO-IFO, c) BSO-BFO; N Leaching d) iSO-iFO, e) ISO-IFO, f) BSO-BFO; and NH_3 volatilization g) iSO-iFO, h) ISO-IFO, i) BSO-BFO. The red-dashed line shows the average difference across 30 years.

To describe the simulated changes in N loss for selected changes in management six tables are presented, one for each site and soil type (Tables 5.2, 5.S6-5.S10). Management impacts which are commonly studied experimentally are presented. As shown in Table 5.2, when changing management from iFO to iSO, NO_3^- leaching on average across 30 years was reduced by 13.4 kg N ha^{-1}, with reductions ranging from -28.3 to -2.5 kg N ha^{-1}. Reduced N leaching occurred across all 30 climate years. Total reactive N was reduced under injected and incorporated slurry application, but often not under broadcast. This was also the case at Woodslee (Table 5.S8, 5.S9) but not for Alfred (Table 5.S6, 5.S7) where reactive N loss was reduced for all three methods of slurry application. At the warmer Gilmore City and Woodslee sites NH_3 volatilization was greater than at Alfred and the benefit of reducing N leaching, runoff and N_2O emissions in broadcast spring organic fertilization was offset by the greater NH_3 losses.

To further quantify differences among management practices, additional tables are provided that show the significant difference among management practices at each location (Tables 5.S11, 5.S12, 5.S13). Average N leaching, N runoff, N_2O emission, NH_3 volatilization, dry silage yield, and reactive N are also provided across the 30 yr of climate variability. Regarding fall versus spring organic fertilization, N leaching was found to be the only reactive N component that was significantly different across all sites and soil textures. Nitrous oxide was significantly different across all application methods and soils at Gilmore City and under the sandy loam at Alfred. Ammonia was always significantly different for broadcast fertilizer application across all sites and soil textures, and also for injected and incorporated sandy loam at Gilmore City and incorporated sandy loam at Woodslee.

Table 5.2 Simulated average change in N loss, maximum and minimum change in any given year, and number of years losses are reduced or increased between selected management scenarios over 30 years of climate variability for clay loam soil at Gilmore City (kg N ha^{-1})

		Injected					**Incorporated**					**Broadcast**				
		Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N
FO to SO	Average	-13.40	-0.01	0.61	-1.41	-14.21	-12.00	-2.31	1.41	-2.85	-15.75	-20.78	-4.03	34.62	-3.87	5.94
	Minimum	-28.31	-0.12	0.11	-3.42	-27.74	-26.00	-4.61	-3.95	-5.40	-31.30	-45.00	-7.69	8.83	-8.13	-26.23
	Maximum	-2.50	0.03	1.26	-0.36	-2.89	1.92	-1.24	7.11	-1.27	-1.88	-4.98	-1.80	58.88	-1.82	34.25
	Lower loss*	30	10	0	30	30	29	30	3	30	30	30	30	0	30	12
	Higher loss*	0	16	30	0	0	1	0	27	0	0	0	0	30	0	18
SO to SM	Average	0.43	-0.02	-0.61	-0.25	-0.45	0.33	-0.04	2.05	0.25	2.59	-1.73	-0.02	-4.11	-0.05	-5.91
	Minimum	-0.74	-0.06	-1.10	-1.06	-1.86	-1.42	-0.07	-6.78	-0.25	-5.89	-4.62	-0.12	-46.08	-0.78	-49.55
	Maximum	4.37	0.02	-0.30	0.17	3.84	4.64	0.05	10.94	0.62	10.69	1.80	0.04	19.81	0.33	17.31
	Lower loss	14	21	30	22	24	13	28	11	5	8	28	21	20	15	22
	Higher loss	15	2	0	7	6	17	1	18	25	22	2	2	10	15	8
SM to SdM	Average	-2.49	0.00	-0.01	0.31	-2.19	-2.29	0.00	-0.97	0.18	-3.07	-1.51	-0.03	-9.77	-0.05	-11.36
	Minimum	-5.86	-0.01	-0.24	-0.27	-6.35	-5.43	-0.01	-9.56	-0.27	-14.55	-5.68	-0.16	-60.84	-0.68	-61.88
	Maximum	-0.29	0.04	0.23	0.88	0.19	1.13	0.05	7.75	0.68	6.71	1.88	0.01	34.12	0.22	30.05
	Lower loss	30	1	12	5	29	29	3	17	4	22	27	28	18	15	18
	Higher loss	0	4	11	25	1	1	5	12	26	8	3	1	12	15	12
SM to SpM	Average	-1.56	0.00	-0.12	0.20	-1.48	-1.15	0.00	-3.71	0.15	-4.71	1.21	-0.02	-16.99	-0.02	-15.81
	Minimum	-3.70	-0.01	-0.37	-0.19	-4.25	-3.22	-0.01	-12.70	-0.16	-15.12	-1.49	-0.11	-45.39	-0.52	-45.45
	Maximum	-0.18	0.03	0.00	0.56	-0.08	1.73	0.07	2.19	0.42	1.77	7.93	0.04	10.07	0.42	10.92
	Lower loss	30	2	20	5	30	28	1	21	5	29	8	23	27	13	29
	Higher loss	0	4	0	25	0	2	6	1	25	1	22	3	3	17	1
SO to SpO	Average	-1.57	0.00	1.30	0.13	-0.13	-2.03	-0.01	3.01	0.19	1.16	3.84	0.01	8.08	0.34	12.26
	Minimum	-3.41	-0.02	0.62	-0.61	-2.49	-5.66	-0.03	-2.89	-0.06	-5.05	0.71	-0.01	-10.55	0.07	-7.15
	Maximum	-0.42	0.01	1.93	0.54	1.91	-0.28	0.00	13.65	0.62	10.44	8.02	0.06	22.20	0.74	26.63
	Lower loss	30	4	0	6	16	30	23	3	4	12	0	5	5	0	3
	Higher loss	0	5	30	23	14	0	0	27	26	18	30	15	25	30	27
Application method		**ISM to iSM**					**BSM to iSM**					**BSM to ISM**				
	Average	0.26	0.00	-4.12	0.14	-3.71	7.84	-0.02	-52.54	0.67	-44.05	7.58	-0.03	-48.42	0.53	-40.34
	Minimum	-0.43	-0.01	-12.33	-0.12	-10.88	0.87	-0.09	-90.13	-0.01	-80.22	0.86	-0.09	-81.35	-0.01	-71.80
	Maximum	2.10	0.03	0.00	0.46	0.03	19.95	0.25	-16.16	1.75	-11.40	18.81	0.24	-5.11	1.70	-0.52
	Lower loss	13	1	21	5	28	0	23	30	1	30	0	24	30	2	30
	Higher loss	16	6	0	24	2	30	5	0	29	0	30	5	0	28	0

i-injected; I-incorporated; B-broadcast; M-mineral; O-organic; S-spring; F-fall; Sd-sidedress; Sp-split
*Number of years that each N component is lower or higher out of the 30 years of weather simulated for the respective change in fertilizer management.

5.3.3.2 Organic versus mineral fertilizer

The overall impact of changing from organic to mineral fertilizer was found to differ across sites, soils and application method. At Alfred, predicted total reactive N loss generally increased when changing management from spring organic to spring mineral fertilization in the clay soil, but the difference was small (Supplemental Table S6). On the other hand, reactive N loss decreased when changing from spring organic to spring mineral fertilization in the sandy loam, with less N leaching and lower NH_3 emissions from spring mineral fertilization, particularly under broadcast (Table 5.S7). A sandy soil is more aerated and DNDC simulates greater rates of decomposition of manure resulting in more $NH4^+$ formation with higher potential for NH_3 volatilization. A similar, yet more pronounced result was seen at Woodslee (Table 5.S8, 5.S9) and Gilmore City (Table 5.2, 5.S10). At the Gilmore City location NH_3 volatilization from the sandy loam was significantly higher from organic than from mineral fertilizer in 4 out of 6 cases (Table 5.S13). Average N_2O emissions were higher from organic amendments across all locations and soil types with significant differences for a few practices at each location (Tables 5.S11, 5.S12, 5.S13), which is consistent with some experimental studies (Schwager et al., 2016; Kramer et al., 2006). In the DNDC model denitrification is driven by availability of both soil N and DOC and DOC is higher under manure application after mineralization of organic matter. Note, however, that across the 30 years DNDC sometimes predicts more N_2O from mineral than organic fertilizer, depending on yearly weather patterns. Interestingly, N leaching or runoff was never found to be significantly different between organic and mineral fertilizer. Varying result have been found from experimental studies where, for example, Svoboda et al. (2013) found higher N leaching losses from mineral than organic fertilizer whereas Kramer et al. (2006) found greater N leaching for organic applications, likely due to enhanced denitrification from higher C inputs.

5.3.3.3 Spring mineral versus side dress mineral

Research has found that sidedress mineral fertilization can improve crop N uptake and yields in comparison with spring application; however, this may only occur if the crop is under N stress (Zebarth et al., 2001). With sidedress mineral fertilization, N application timing corresponds better with crop N demand, being at about the sixth-leaf stage for corn silage. Overall, model simulations indicate that sidedress mineral fertilization reduced N loss and slightly increased biomass. In situations where crop N stress was high such as at Gilmore City, (Table 5.2, S10) , difference in silage yield response was more pronounced (~3% greater). The higher crop N stress at Gilmore City was due to higher NH_3 volatilization losses as a result of higher temperatures than at Alfred and higher soil water availability during the growing season (Fig. 5.S1) than at Woodslee, both of which are drivers that increase volatilization in DNDC (Dutta et al., 2016a).

5.3.3.4 Spring mineral versus split mineral

Interestingly, split mineral fertilization reduced N loss more than sidedress mineral fertilization (Tables 5.2, 5.S6-5.S10). This was primarily because NH_3 emissions at the sixth leaf stage application were usually lower than under sidedress mineral fertilization. Urea hydrolysis increases OH^- concentration in the soil, enhancing NH_3 volatilization (Dutta et al., 2016a). In the case of sidedress mineral fertilization, relative to split mineral fertilization, more urea is applied in the warmer portion of the year. This alone enhances NH_3 loss, but also the soil pH shift is larger due to more urea undergoing hydrolysis at this higher temperature. As an average across sites, split fertilizer reduced reactive N per metric ton of dry silage by 6.4, 8.8, and 12.0% in the sandy loam for injected, incorporated, and broadcast applications, respectively, whereas it was reduced by 1.9, 6.0 and 21.5% in the clay loam. At all locations and in all soils, except for the Alfred clay, silage yields were marginally higher for split mineral fertilization than under spring mineral fertilization (Tables 5.S11, 5.S12 and 5.S13). Average yield over 30 yr was, in fact, 8.9% higher for split mineral fertilization for the sandy loam broadcast treatment at Gilmore City; however, this was still not significant at the 0.05 level.

5.3.3.5 Spring organic versus split organic

For all locations and soil textures, split organic fertilization reduced N leaching under the injected and incorporated treatments but increased N leaching when broadcast (Tables 5.2, 5.S6-5.S10). In the model this is caused by a higher rate of decomposition, and nitrification near the soil surface for broadcast manure at higher temperatures resulting in more N available for leaching. Because of increased decomposition rates of the manure applied at sixth-leaf stage, split organic fertilization usually produced greater N_2O and NH_3 volatilization than spring organic fertilization. This resulted in a tradeoff in losses between N leaching and N_2O or NH_3 when fertilizer was injected or incorporated.

5.3.3.6 Application method

We examined the differences in reactive N losses between injected, incorporated and broadcast application methods for spring applied urea across all sites and soils and the outcome was clear (Tables 5.2, 5.S6-5.S10). In at least 28 of 30 yr, more reactive N loss occurred under incorporated than under injected application. When comparing broadcast with injected or incorporated applications, more losses occurred in all 30 yr for broadcast treatments.

5.3.4 Comparative analysis of simulated reactive N losses between locations and soil types

Reactive N as a sum of N leaching, N runoff, N_2O-N and NH_3-N is analysed per ton of dry harvested silage in Fig. 5.4. Although this summation may undervalue the importance of specific reactive N components (i.e. N_2O which has a large global warming capacity) it provides a good metric of the overall performance of the system to retain N which is of economic consequence to farmers. This figure provides an aggregated synopsis of the outcomes from the entire study. There are several clear trends demonstrated which align with results from experimental studies. There is more reactive N loss from the coarser texture sandy loam, more N losses occur for broadcast, followed by incorporated in comparison to injected fertilizer application, and a little more overall average N loss occurs from organic than mineral fertilizer. The sandy loam soil texture resulted in 2.6, 1.8 and 3.0 times more reactive N loss per metric ton of silage biomass than did the finer textured soils at Alfred, Woodslee and Gilmore City, respectively. Silage biomass was reduced on average by 18, 35, and 16% for the sandy loam soils in comparison to clay soils at Alfred, Woodslee, and Gilmore City, respectively (Table 5.S11, 5.S12, 5.S13). This was due to increased crop water and N stress for the sandy loam soils relative to the clay soils. Although annual precipitation was similar between Woodslee and Gilmore City sites more crop water stress was predicted to occur under the sandy loam soil at Woodslee due to less precipitation during the growing season (Fig. 5.S1) and greater runoff in the non-growing season. Overall, the sandy loam soils showed more consistency in the ranking of fertilizer managements across sites than did the clay textured soils. This is because coarser textured soils are more susceptible to N loss and related crop N stress thus management that is beneficial for reducing N loss has more influence.

Regarding the timing of fertilizer application, sidedress and split application are recommended for reducing reactive N loss, and fall application should be avoided. On average across the sites, fall-applied manure in comparison with spring-applied manure increased reactive

N loss per metric ton of silage by 109, 109, and 27% for injected, incorporated, and broadcast application, respectively, on sandy loam soils. Likewise reactive N per metric ton of silage for fall-applied manure in comparison with spring-applied manure was increased by 43, 44, and 14%, for injected, incorporated, and broadcast application on clay soils. Silage biomass was not significantly affected by the increased N losses during the fall in the clay soils; however, biomass under fall organic relative to spring organic in the sandy loam soils was reduced by 26 and 29% for the Alfred and Woodslee sites, respectively (Table 5.S11, 5.S12). Interestingly, there was no change in simulated biomass after fall manure application at Gilmore City, but it has been suggested that N mineralization is high at this site at ~140.4 kg N ha^{-1} y^{-1} for a corn-soybean [Glycine max (L.) Merr.] rotation (Qi et al., 2011b). The DNDC model simulated, on average, 79, 114, and 139 kg N ha^{-1} yr^{-1} of mineralization at Alfred, Woodslee, and Gilmore City, respectively.

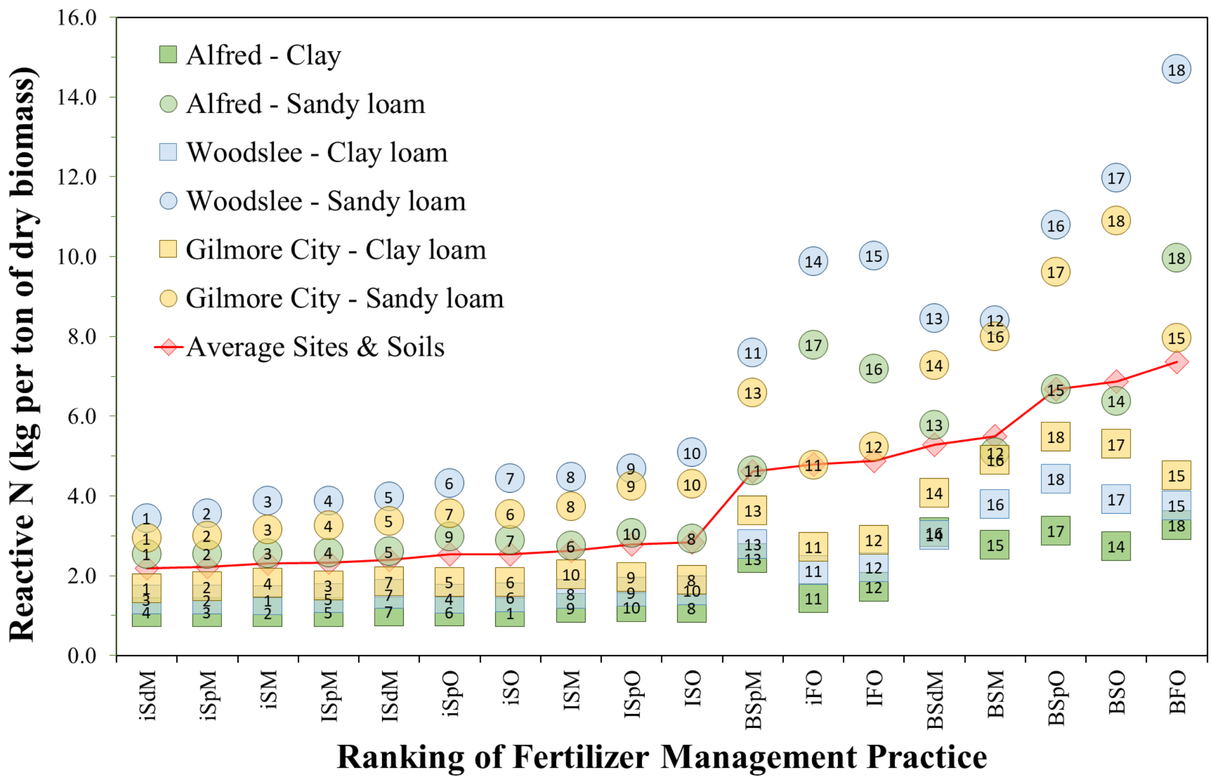

Figure 5.4. Average reactive N (sum of N leaching, N runoff, N_2O-N and NH_3-N) per ton of dry harvested silage over 30 years for each location, soil type and fertilizer management practice. i-injected; I-incorporated; B-broadcast; M-mineral; O-organic; S-spring; F-fall; Sd-sidedress; Sp-split. The number at each data point signifies the ranking of the fertilizer management practice for each site and soil type.

5.4 Conclusions

In this study a well-tested DNDC model version, with recently integrated mechanistic tile drainage, was used to investigate the impacts of N loss from 9 organic and 9 inorganic fertilizer management practices across 3 locations and 30 years of climate variability. Similar impacts of fertilizer management were often determined between locations and these were highly variable across climate but usually agreed with observations. Reactive N losses were much greater from coarser than the finer textured soils and in many cases climate variability had more influence on reactive N loss than did changes in fertilizer management. There was much greater reactive N loss from fall-applied than from spring-applied manure slurry, and the most beneficial managements were shown to be injected split and sidedress mineral fertilizer. Several on farm management decisions come into play when considering fertilizer application method. These can include fertilizer source and type of equipment available for application, manure storage considerations, and on farm time management between multiple tasks. The results presented in this study can be used to guide producers in planning fertilizer management in an effort to reduce N loss, and minimize the environmental footprint.

5.5 Supplementary Sections, Tables and Figures

Section 5.S1 Description of experimental sites

Alfred, Ontario, Canada

A 2.5 year experimental study (years 2011-2014) was initiated in October 2011 at Alfred, Ontario (45.34° N, 74.55° W) on a tile-drained Bearbrook clay (47% clay, 18% silt) and is classified as an Orthic Humic Gleysol. Fertilizer treatments included raw and digested manure applied in either the fall or spring, as well as an inorganic fertilizer (urea) applied in the spring, along with control plots (no fertilizer). All treatments were initially broadcast and then shortly incorporated with a targeted application rate of 140 kg N ha^{-1}. The manure application N rate was determined by using factors for total ammoniacal N (TAN) retention and organic N mineralization. All treatments were seeded to silage-corn. Direct N_2O emissions, NO_3 in tiles, soil N, and crop measurements were conducted over the study period. Please see Schwager et al. (2016) for a more detailed description of soil, management and experimental setup.

Woodslee, Ontario, Canada

The initial field study was conducted on a field that was previously established in 1991 to monitor surface runoff and tile drainage. It is located on a farm at Woodlsee, Ontario (42°13'N, 82°44'W) on a Brookston clay-loam, and is classified as an Orthic Humic Gleysol. The research study focused on was of 5 years duration (years 2000-2005) for a corn-soybean rotation with and without a winter wheat cover crop, with measurements of water volume and N concentrations to tile drains and to runoff. Both a starter (18-46-0) and sidedress application of UAN (150 kg N ha^{-1}) was applied to corn for a combined nitrogen rate of 175 kg N ha^{-1}. Corn grain was harvested in early November and tillage generally consisted of fall disking except when excessive residue required a more substantial cultivated heavy plough. Measurements include water and NO_3 to tiles, soil mineral N, crop biomass and yield measurements. Please see Drury et al. (2014b) for a more detailed description of soil, management and experimental setup.

Gilmore City, Iowa, USA

A five year field experiment was established in the fall of 2004 at the Agicultural Drainage and Water Quality – Research and Demonstration Site close to Gilmore City in north central Iowa, USA (42_420N 104_000W). The region is predominantly made up of the following soils; Nicollet (fine-loamy, mixed, superactive Aquic Hapludoll), Webster (fine-loamy, mesic Typic Endoaquolls), Canisteo (fine-loamy, mesic Typic Endoaquolls), and Okoboji(Fine, smectitic, mesic Cumulic Vertic Endoaquolls). Four land cover treatments were initiated consisting of winter rye growth prior to corn and prior to soybean – first phase of the rotation (TRT1), winter rye cover crop growth prior to soybean and prior to corn – second phase of the rotation (TRT2), corn and soybean without cover crop –first phase of rotation (CTRL1) and corn and soybean without cover crop –second phase of rotation (CTRL2). Aqueous ammonium nitrogen was applied to corn at a rate of 140 kg N ha^{-1} in the spring near emergence time. The site includes a larger compliment of measurements including water content at 4 depths, biomass and crop N uptake and daily measurement of water flow and N concentration to tile drains. Please see Qi et al. (2011a) for a more detailed description of soil, management and experimental setup.

Section 5.S2 Description of N loss processes in Canada DNDC

Nitrous oxide emissions

In DNDC nitrification and denitrification processes are characterized in the “anaerobic balloon” sub-model. The “anaerobic balloon” concept uses the Nernst equation to estimate redox potential (Eh) which regulates the size of the anaerobic (denitrifier) and aerobic (nitrifier) microbial fractions. The anaerobic portion is considered to be inside the balloon and the aerobic outside. The nitrification rate is determined as a function of nitrifier bacteria biomass, NH_4^+ concentration, a temperature reduction factor, a moisture reduction factor and pH. The N_2O from nitrification is regulated by water filled pore space, quantity of N nitrified, and temperature. In addition to determining when nitrification and denitrification occurs the Nersnt equation determines when specific biologically mediated reductive identification reactions occur, from $NO_3 \rightarrow NO_2 \rightarrow NO \rightarrow N_2O \rightarrow N_2$. The rate of the reactions (microbial growth) is then determined using the Michaelis–Menten equation, a multi-nutrient dependent growth function dependent on temperature, dissolved organic carbon, soil water, Eh, and pH. N_2O from denitrification is calculated as stepwise transformation process as a function of microbial growth and pH.

NH_3 volatilization

In DNDCv.Can a new sub-model which operates on an hourly time step was included by Congreves et al. (2016b) to improve the simulation of NH_3 volatilization. This sub-model is based on chemical equilibria principles whereby the acid–base equilibrium between NH_4^+ and NH_3 is determined in aqueous solution with the reaction rates being determined by the pH of the mixed soil solution and the dissociation constants influenced by soil temperature. NH_4^+ adsorption by clay in the model also restricts mobility and limits availability for the acid-base equilibrium. The aqueous-gas equilibrium is then calculated using Henry’s law with NH_3 volatilization being limited by a soil depth function. The utility of this development was further improved by Dutta et al. (2016a) who improved the simulation of urea hydrolysis and included the impact of buffer capacity on soil pH. Urea hydrolysis is determined as a function of N-urea concentration, volumetric moisture content, and a kinetic rate constant for hydrolysis. The pH buffering was derived from Tripathi et al. (2000) and is primarily a function of the cation exchange capacity of the soil.

N leaching

The hydrological framework in DNDCv.Can was recently enhanced (Chapter 4) by including a new mechanistic tile drainage sub-model and root growth dynamics. The water flux mechanisms were also improved and a deeper and heterogeneous soil profile was included. These developments improved the simulation of available N in the profile since mineralization, clay adsorption, denitrification and nitrification were simulate over 200 cm depth rather than only 50 cm in the default model version. The original nitrate movement in DNDC was conceived as firstly a function of the water flux per layer. Soil nitrate was considered to be mobilized by a positive water flux (90% mobilized) and transferred to the layer below as a one-dimensional vertical N flux towards the bottom soil profile. The movement of N is an iterative step through each of the saturated layers per hour that are drained to tiles. Note that nitrification followed by NH_4^+ adsorption to clay also restricts N mobility since there is less NO_3^- available in solution. Additionally, another fraction (10% of the NO_3^- in each layer) was considered to be lost through preferential water flow via macropores directly out of the soil profile. In DNDCv.Can this preferential N loss function was modified to ensure correlation with water movement. It was found that DNDC sometimes simulated N movement when there was no water flow. In DNDCv.Can the fraction of NO_3^- available to be transferred to the layer below at an hourly time step can now be parameterized through the user interface with a default value of 0.9. The fraction per layer that is preferentially lost directly to drains is set to a default fraction of 0.02. Nitrate tile losses to tiles are calculated starting from the layer situated at the top of the water table down to the layer at the bottom of the tile drains.

N runoff

For estimating runoff DNDC uses the SCS runoff curve number method developed by the USDA Natural Resources Conservation Service. Smith et al. (2019c) found that for default DNDC nitrate losses to runoff were very low for all cropping systems. To address this issue we first fixed a water mass balance error in the SCS runoff curve number method. Second, the model was greatly modified to simulate a fluctuating water table and when the water table reaches the soil surface runoff and additional loss of N could then occur. Further, N loss to runoff was originally calculated as a fraction of rainfall that goes to runoff (based on SCS method) multiplied by the nitrate found in only the top surface layer (~0.5 - 2 cm). We extended this calculation to the top 2 layers and included a user defined parameter where the fraction can be adjusted.

Section 5.S3 Model validation for simulating drainage and N loading to tiles at Alfred, Woodslee and Gilmore City

To evaluate model performance, several statistics were employed to compare simulations against measurements including normalized average relative error (NARE), Nash-Sutcliffe efficiency (NSE), and index of agreement (d) (Nash and Sutcliffe, 1970; Willmott, 1985). Based on the recommendations in previous studies (Moriasi et al., 2007; He et al., 2018b), a NSE ($-\infty$ to 1) value=1.0 indicates "perfect" agreement, NSE>0.5 indicates "good" agreement, NSE>0.0 indicates "fair" agreement, and a NSE<0.0 indicates "poor" agreement between simulated and measured data. A value of d≥0.9 illustrates "excellent" match, 0.8≤d<0.9 illustrates "good" match, 0.7≤d<0.8 illustrates "fair" match, and d<0.7 illustrates "poor" match when comparing the simulated and measured values.

At the Alfred site cumulative drainage and N loading was very well simulated by the revised model (He et al., 2019b), but capturing the timing of daily water flow and monthly N loss to tile drains was more problematic (Tables S2, S3). In all cases the model produced a "fair" simulation. At this site the snow cover dynamics and freeze-thaw events during the winter, particularly in the 2013-2014 year were complex. DNDC is a 1-D model thus for instances where there was significant blowing snow the effect of snow insulation may not be well simulated. This resulted in a fair simulation of daily water and N dynamics, however, the simulation of water flow was improved over Guest et al. (2018) who compared DNDC to the water budget models HOLOS and VSMB. In Guest et al. (2018) DNDC performed better than HOLOS and VSMB but under-predicted drainage by 33% with an RMSE of 76 mm whereas the revised model in this study under-predicted by 3-11% (Table S2) with an RMSE of 35.7 mm.

In general, the revised model performed very well at both the Woodslee and Glimore City sites where predicted water loss to tiles was simulated with NSE>0.5, except at for the control drained, no-cover crop treatment at Woodslee where observations were much lower than the cover crop treatment. In all cases simulations were improved over default DNDC (Table S2). This is not surprising since the model previously only simulated bulk flow of water with no tile drainage algorithm. Note that the pre-developed model was not capable of simulating controlled drainage or sub-irrigation. At the Woodslee site N loss to tiles was well simulated for the cover crop and no-cover crop treatments with conventional tile drainage but the timing of N loss was not as well simulated for the control drained, sub-irrigated treatments (Table S3). Note the cumulative N losses to drains was well simulated with the appropriate reduction in losses under controlled drainage (Observed 38.3%; DNDC 37.4%). N loss to tiles was predicted with "excellent" accuracy for all treatments at Gilmore City. Note that N concentrations in tile drainage were measured less frequently that water volumes.

Additionally, it was found that revised DNDC model performed similarly to RZWQM2 for simulating average daily drainage across the validation treatments (NSE~0.6), and better for simulating N loading to drains (NSE, DNDC: 0.72, RZWQM2: 0.54) and soil water storage (NSE, DNDC: 0.34, RZWQM2: -0.19). Simulation of drainage and N loading were on average better simulated at the Woodslee site. This demonstrated that DNDC development was successful considering RZWQM2 is a well-validated water quality model which includes detailed computational hydrology.

Section 5.S4 Model validation for simulating corn silage biomass and N uptake, soil N and N_2O emissions at Alfred

At the Alfred site the model indicated excellent performance based on the average statistical values of d index (d>0.90), Nash-Sutcliffe efficiency (NSE>0.5) and normalized average relative error (NARE<20%) for biomass, N uptake, and annual N_2O emissions (Table S4). Soil N was also well simulated with good to excellent performance based on d>0.80. See He et al. (2019b) for further details.

Section 5.S5 Comparison of simulated 30 year average model outcomes to measurements at Alfred

Most of our model inputs and parametrization for manure, urea and corn silage were based on the Alfred site, thus it is useful to compare the general simulation results across our 30 year analysis to site observations. Note that there were differences between site-specific and modelled management history. At Alfred, N_2O emissions from corn silage, treated with raw manure slurry in the spring and fall and urea in the spring, were measured from the fall of 2011 until the spring of 2014. Simulated N_2O emissions over 30 years from incorporated raw manure, averaged across fall and spring applications (4.3 kg N $ha^{-1}y^{-1}$), were relatively similar to observed average annual emissions (4.9 kg N ha^{-1} y^{-1}) (Schwager et al., 2016). The simulated annual emissions ranged from 3.0 to 10.5 kg N $ha^{-1}y^{-1}$ for IFO and 2.8 to 9.8 kg N $ha^{-1}y^{-1}$ for ISO indicating that there may be large inter-annual variability depending on weather patterns. The trends in simulated N_2O emissions, and also NO_3^- leaching, agreed well with observations with greater losses occurring in the fall relative to spring. Measurements showed that spring applied organic and mineral fertilizer produced similar emissions across the 2 study years, however, the model showed more average emissions across the 30 years from the manure (Table S11, S12 and S13). This was true for all methods of application, soil types, and study locations. Similar to Schwager et al. (2016) greater water and N loss to drains was simulated in the non-growing season as compared to the growing season. Schwager et al. (2016) found that the 6-7 kg ha^{-1} more N leaching occurred for manure applied in fall compared to spring. Over the same years we simulated 5 kg ha^{-1} more N leaching in the fall. Non-growing season N_2O emissions from the manure slurry were simulated to be 17% of annual emissions when spring applied and 51% when fall applied, as an average over 30 years, versus 29% and 68%, respectively determined from observations over 2 years (Schwager et al., 2016). A detailed comparison, employing identical site management, of modelled and simulated drainage and N loading to tiles is provided in supplementary material.

The observed biomass for ISM, ISO and IFO for the years 2012-2013 were 17055, 13454 and 14138 kg ha^{-1}, respectively whereas the modelled estimates over the same two years were 13551, 13595, and 13563, respectively, with reduced yields driven by water stress for each treatment, rather than N stress. It was a particularly dry year in 2012 and 2013 was dryer than average. There is a known issue in the clay field where water table level was significantly higher in northern plots which may have reduced crop water stress and impacted yields under ISM management (Schwager, 2015). The modelled averages over the 30 years were 15747, 15239, and 14937 for ISM, ISO and IFO, respectively.

Table 5.S1 Soil characteristics at Alfred, Gilmore City and Woodslee research plots

Location and data collection period	Soil classification*	Average annual temp. (°C)	Average annual Precip. (mm)	Soil characteristics: Soil surface texture (%)	SOC ($g\ kg^{-1}$)	pH	Bulk density ($g\ cm^{-3}$)
Alfred, Ontario, Canada 45.34° N, 74.55° W (2011-2014)	Orthic Humic Gleysol	4.5	1021	35 sand 18 silt 47 clay	23.2	7.1	1.34
Woodslee, Ontario, Canada 42°13'N, 82°44'W (1999-2005)	Orthic Humic Gleysol	9.8	816	28 sand 35 silt 37 clay	25.0	7.0	1.42
Gilmore City, Iowa, United States 42°42'N 104°00'W (2005-2009)	Nicollet (fine-loamy, mixed, superactive, mesic Aquic Hapludoll)	8.7	824	32 sand 34 silt 32 clay	23.2	7.1	1.37

* Other soil series are also present at the Gilmore City site.

Table 5.S2 Statistical performance of DNDC for simulating water flow to tile drains in cool weather climates

Site	Calibration		Validation					
	Default DNDC	Revised DNDC	Default DNDC	Revised DNDC	Default DNDC	Revised DNDC	Default DNDC	Revised DNDC
Alfred Ontario (daily)								
	Control		Urea		Spring manure		Fall manure	
NARE	NA	-3.12	NA	-11.4	NA	-6.86	NA	-6.24
NSE	NA	0.14	NA	0.27	NA	0.09	NA	0.13
d	NA	0.74	NA	0.77	NA	0.73	NA	0.70
Woodslee, Ontario (n=28 over 5 years)								
	CC		NCC		CC, CD-SI		NCC, CD-SI	
NARE	9.5	-0.5	-0.5	12.7	NA	-1.9	NA	39.8
NSE	-0.13	0.87	-0.06	0.83	NA	0.77	NA	0.20
d	0.67	0.96	0.82	0.96	NA	0.95	NA	0.84
Gilmore City, Iowa (daily)								
	CC, Corn-Soy		NCC, Corn-Soy		CC, Soy-Corn		NCC, Soy-Corn	
NARE	1.6	3.8	-5.3	-4.7	-16.1	-17.0	17.5	16.6
NSE	-0.32	0.55	0.08	0.51	0.24	0.59	-0.11	0.70
d	0.68	0.82	0.72	0.76	0.74	0.81	0.67	0.88

*Alfred statistics are summarized from He et al. (2019), Woodslee and Gilmore City from unpublished data.
CC – cover crop; NCC – No cover crop; CD-SI – controlled drainage and subsurface irrigation; Corn-Soy – Corn-soybean rotation beginning with corn

Table 5.S3 Statistical performance of DNDC for N loss to tile drains in cool weather climates

Site	Calibration		Validation					
	Default DNDC	Revised DNDC	Default DNDC	Revised DNDC	Default DNDC	Revised DNDC	Default DNDC	Revised DNDC
Alfred Ontario (monthly)								
	Control		Urea		Spring manure		Fall manure	
NARE	NA	36.0	NA	4.4	NA	21.8	NA	34.7
NSE	NA	0.17	NA	0.26	NA	0.06	NA	0.16
d	NA	0.79	NA	0.73	NA	0.75	NA	0.74
Woodslee, Ontario (n=28 over 5 years)								
	CC		NCC		CC, CD-SI		NCC, CD-SI	
NARE	23.6	-0.3	14.7	10.8	NA	10.3	NA	3.6
NSE	0.35	0.55	0.56	0.63	NA	0.11	NA	-0.20
d	0.79	0.80	0.83	0.88	NA	0.66	NA	0.60
Gilmore City, Iowa (monthly)								
	CC, Corn-Soy		NCC, Corn-Soy		CC, Soy-Corn		NCC, Soy-Corn	
NARE	7.4	8.9	-3.0	-0.5	-10.7	-3.1	14.1	11.7
NSE	0.53	0.69	0.65	0.77	0.59	0.75	0.58	0.64
d	0.85	0.92	0.89	0.93	0.82	0.93	0.86	0.92

*Alfred statistics are summarized from He et al. (2019), Woodslee and Gilmore City from unpublished data.
CC – cover crop; NCC – No cover crop; CD-SI – controlled drainage and subsurface irrigation; Corn-Soy – Corn-soybean rotation beginning with corn

Table 5.S4 Model validation for simulating corn silage biomass, corn silage N uptake, soil N and annual N_2O emissions from manure slurry and urea at Alfred.

Item	Calibration			Validation								
	Control			Urea			Spring manure			Fall manure		
	NARE	NSE	d	NARE	NSE	d	NARE	NSE	d	NARE	NSE	d
Above-ground biomass	-1.2	0.89	0.98	-9.0	0.91	0.98	10.2	0.71	0.93	16.7	0.79	0.96
Crop N uptake	9.8	0.74	0.96	-7.4	0.95	0.98	12.7	0.98	0.98	17.0	0.87	0.97
Soil NO_3^- (0-15 cm)	-19.9	0.48	0.83	24.3	0.84	0.97	-38.4	0.41	0.89	-48.2	0.38	0.82
Annual N_2O emissions	-12.7	0.81	0.96	12.7	0.74	0.94	-19.8	0.63	0.91	-5.6	0.98	0.99

The statistics are summarized from He et al. (2019b).

Table 5.S5 DNDC model parameters, observed from local studies, default and calibrated

Sites	Alfred Clay	Alfred Sandy Loam	Iowa Clay Loam	Iowa Sandy Lam	Woodslee Clay Loam	Woodslee Sandy Loam
Crop Parameters						
Grain fraction	0.40*^	0.40	0.40	0.40	0.40	0.40
Stem+leaf fraction	0.48*	0.48	0.48	0.48	0.48	0.48
Root fraction	0.12*	0.12	0.12	0.12	0.12	0.12
Grain C:N	35*	35	35	35	35	35
Stem+leaf C:N	55*	55	55	55	55	55
Root C:N	60*	60	60	60	60	60
Water requirement	70*	70	70	70	70	70
GDD (0^{o}C base)	2300*	2300	2300	2300	2300	2300
Soil Parameters#						
Litter fraction	0.01+	0.01+	0.01+	0.01+	0.01+	0.01+
Humads fraction	0.025+	0.025+	0.09*	0.025+	0.095*	0.025+
Humus fraction	0.965+	0.965+	0.90*	0.965+	0.895*	0.965+
Organic C (%)	2.6	1.5	2.5	1.5	2.5	1.5
Field capacity (WFPS)	0.72	0.40	0.80	0.40	0.815	0.40
Wilting point (WFPS)	0.49	0.185	0.44	0.185	0.562	0.185
KSat (m/hr)	0.015	0.1248	0.0382	0.1248	0.020	0.1248
Tile Drainage Factors#						
Tile spacing (m)	15.0	30.0	7.6	30.0	7.5	30.0
Drain radius (m)	0.01	0.01	0.0768	0.01	0.01	0.01
Tile depth (m)	0.9	1.4	1.06	1.4	0.65	1.4
Lateral Ksat to drains (multiplier of vertical Ksat)	1.8*	1.8	1.8*	1.8	1.8*	1.8

*calibrated parameters

^The same silage cultivar that was calibrated to simulate appropriate biomass and N uptake at Alfred was employed in DNDC across all sites and soils

+default parameters

#values for sandy loam are estimated (not based on local site values)

Table 5.S6 Simulated average change in N loss, maximum and minimum change in any given year, and number of years losses are reduced or increased between selected management scenarios over 30 years of climate variability for the clay soil at Alfred (all results in kg N ha^{-1})

		Injected					Incorporated					Broadcast				
		Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N
FO to SO	Average	-5.30	0.02	0.14	-0.27	-5.40	-4.34	-2.70	-0.07	-0.49	-7.60	-7.70	-9.46	9.07	-1.13	-9.22
	Minimum	-11.27	-0.02	0.04	-1.60	-11.03	-10.60	-6.79	-4.72	-1.72	-14.65	-14.41	-21.97	-14.76	-3.11	-35.76
	Maximum	1.78	0.16	0.29	0.34	1.90	2.01	-1.00	0.61	0.77	0.31	1.31	-4.05	23.39	-0.02	12.69
	Lower loss*	28	2	0	21	29	27	30	4	25	29	29	30	5	30	26
	Higher loss*	2	24	30	9	1	3	0	26	5	1	1	0	25	0	4
SO to SM	Average	1.00	-0.01	-0.19	-0.37	0.43	0.45	-0.23	0.98	-0.61	0.58	1.60	-0.11	1.17	0.11	2.77
	Minimum	-0.29	-0.04	-0.33	-1.22	-1.46	-1.00	-0.44	-0.66	-1.61	-2.40	-0.47	-0.44	-18.67	-0.81	-15.85
	Maximum	3.66	0.11	-0.10	0.10	3.13	3.49	-0.05	6.29	0.63	4.74	4.14	0.23	19.31	0.68	19.88
	Lower loss	5	22	30	29	12	14	30	20	27	15	2	25	14	13	12
	Higher loss	25	4	0	1	18	15	0	10	3	15	28	5	16	17	18
SM to SdM	Average	-0.29	0.01	0.02	0.44	0.17	-0.28	0.00	-1.11	0.05	-1.34	-0.66	-0.07	5.26	0.39	4.92
	Minimum	-0.87	0.00	-0.11	-0.09	-0.50	-0.99	-0.01	-6.81	-0.73	-6.66	-3.21	-0.42	-37.71	-0.52	-36.26
	Maximum	0.20	0.10	0.24	1.06	0.99	0.95	0.05	1.41	0.71	1.90	2.12	0.41	36.30	1.47	35.94
	Lower loss	25	0	4	2	8	26	4	10	12	21	25	18	13	4	13
	Higher loss	4	7	7	28	22	4	3	7	18	9	5	12	17	26	17
SM to SpM	Average	-0.18	0.00	-0.01	0.28	0.10	-0.15	0.00	-1.34	-0.10	-1.59	0.65	0.02	-6.11	0.43	-5.01
	Minimum	-0.70	0.00	-0.11	-0.06	-0.37	-0.54	-0.02	-6.81	-0.63	-6.85	-0.34	-0.21	-32.01	-0.06	-31.18
	Maximum	0.29	0.06	0.00	0.70	0.59	1.04	0.01	0.00	0.33	0.11	3.26	0.49	14.05	1.24	14.56
	Lower loss	24	0	4	3	11	25	2	10	19	27	5	15	21	2	21
	Higher loss	5	4	0	27	19	5	1	0	11	3	25	15	9	28	9
SO to SpO	Average	-0.37	0.00	0.27	0.31	0.21	-0.69	-0.03	0.50	0.32	0.09	3.30	0.13	4.07	1.21	8.71
	Minimum	-1.15	0.00	0.07	-0.25	-0.56	-1.74	-0.12	0.12	-0.24	-1.13	1.14	-0.14	-10.96	0.74	-6.92
	Maximum	0.30	0.01	0.54	0.63	1.24	0.20	0.07	1.18	1.52	1.58	7.68	0.90	18.97	2.77	23.40
	Lower loss	24	0	0	3	12	28	22	0	5	16	0	9	11	0	3
	Higher loss	6	2	30	27	18	2	7	30	25	14	30	21	19	30	27
Application method		ISM to iSM					BSM to iSM					BSM to ISM				
	Average	0.10	-0.01	-1.32	-0.52	-1.75	0.17	-0.63	-25.37	-1.03	-26.85	0.07	-0.62	-24.04	-0.51	-25.10
	Minimum	-0.34	-0.12	-6.70	-0.83	-7.29	-2.76	-1.15	-50.31	-1.48	-51.49	-2.92	-1.15	-46.18	-0.84	-46.67
	Maximum	1.04	0.00	0.00	-0.23	0.22	2.12	-0.46	-2.00	-0.56	-3.45	1.08	-0.46	-2.00	-0.16	-2.96
	Lower loss	6	6	10	30	29	6	30	30	30	30	7	30	30	30	30
	Higher loss	22	0	0	0	1	24	0	0	0	0	23	0	0	0	0

i-injected; I-incorporated; B-broadcast; M-mineral; O-organic; S-spring; F-fall; Sd-sidedress; Sp-split

*Number of years that each N component is lower or higher out of the 30 years of weather simulated for the respective change in fertilizer management.

Table 5.S7 Simulated average change in N loss, maximum and minimum change in any given year, and number of years losses are reduced or increased between selected management scenarios over 30 years of climate variability for the sandy loam soil at Alfred (all results in kg N ha^{-1})

		Injected					Incorporated					Broadcast				
		Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N
FO to SO	Average	-32.94	0.18	0.71	-0.62	-32.67	-27.57	-4.19	0.80	-0.99	-31.95	-26.88	-8.88	16.83	-1.47	-20.41
	Minimum	-60.17	0.05	0.19	-2.74	-59.50	-48.87	-15.32	-9.76	-3.02	-51.77	-50.31	-26.58	-22.68	-3.19	-68.39
	Maximum	-2.15	0.82	1.44	0.23	-2.22	-1.52	-0.89	5.70	0.20	-2.61	-1.10	-2.28	35.35	-0.43	21.02
	Lower loss*	30	0	0	26	30	30	30	3	28	30	30	30	4	30	24
	Higher loss*	0	30	30	4	0	0	0	27	1	0	0	0	26	0	6
SO to SM	Average	-2.88	-0.21	-0.92	-0.38	-4.39	-1.17	-0.07	-0.61	-0.38	-2.22	-0.21	-0.03	-12.95	-0.19	-13.38
	Minimum	-4.57	-0.51	-1.62	-0.84	-6.51	-3.57	-0.18	-5.90	-1.29	-6.50	-2.70	-0.20	-36.58	-0.48	-37.13
	Maximum	-0.69	-0.08	-0.41	-0.19	-2.74	0.13	-0.01	8.83	-0.11	7.29	2.92	0.28	15.18	0.00	13.42
	Lower loss	30	30	30	30	30	29	30	23	30	25	14	23	25	29	25
	Higher loss	0	0	0	0	0	1	0	7	0	5	16	6	5	0	5
SM to SdM	Average	-0.51	0.02	0.09	0.14	-0.26	-0.97	-0.03	-0.72	0.06	-1.66	-1.50	0.00	10.03	0.11	8.64
	Minimum	-1.49	-0.01	-0.17	0.05	-1.29	-2.45	-0.05	-9.31	-0.16	-10.14	-2.69	-0.32	-25.84	-0.01	-26.04
	Maximum	0.41	0.28	0.78	0.25	0.56	0.21	0.02	3.97	0.25	2.52	0.63	0.64	50.52	0.23	48.90
	Lower loss	29	1	1	0	21	29	27	9	2	21	29	24	7	1	8
	Higher loss	1	11	10	30	9	1	2	10	26	9	1	5	23	29	22
SM to SpM	Average	-0.27	0.01	-0.01	0.09	-0.17	-0.66	-0.04	-1.37	0.01	-2.05	-0.26	0.04	-5.64	0.10	-5.77
	Minimum	-0.95	0.00	-0.17	0.03	-0.79	-1.68	-0.14	-10.88	-0.18	-11.38	-1.28	-0.15	-25.15	0.03	-23.68
	Maximum	0.46	0.18	0.16	0.17	0.59	0.17	-0.01	1.56	0.15	1.22	1.60	0.85	23.99	0.22	23.23
	Lower loss	26	0	2	0	23	29	30	10	9	28	24	13	21	0	21
	Higher loss	3	10	1	30	7	1	0	2	20	2	5	10	9	30	9
SO to SpO	Average	-0.57	0.00	1.57	0.25	1.25	-0.58	-0.01	2.02	0.30	1.74	1.92	0.05	6.60	0.38	8.95
	Minimum	-1.33	-0.02	0.68	0.04	-0.12	-2.33	-0.04	-0.07	-0.22	0.02	0.03	-0.04	-7.11	0.07	-4.36
	Maximum	0.64	0.05	3.06	1.31	3.59	0.39	0.02	9.56	1.32	8.53	6.07	0.81	19.52	1.52	21.04
	Lower loss	26	1	0	0	1	27	17	1	2	0	0	4	9	0	5
	Higher loss	4	9	30	30	29	3	6	29	28	30	30	19	21	30	25
Application method		ISM to iSM					BSM to iSM					BSM to ISM				
	Average	-0.57	-0.06	-1.45	-0.14	-2.23	-1.29	-0.14	-31.86	-0.20	-33.48	-0.72	-0.08	-30.41	-0.05	-31.25
	Minimum	-1.07	-0.59	-10.88	-0.39	-11.43	-4.00	-0.55	-59.75	-0.53	-58.80	-3.15	-0.21	-57.26	-0.18	-55.71
	Maximum	0.42	-0.02	0.00	0.01	-0.48	1.17	-0.07	0.00	-0.09	-4.16	1.53	0.04	0.00	0.03	-3.17
	Lower loss	28	30	10	29	30	28	30	29	30	30	26	28	29	28	30
	Higher loss	2	0	0	1	0	2	0	0	0	0	2	2	0	1	0

i-injected; I-incorporated; B-broadcast; M-mineral; O-organic; S-spring; F-fall; Sd-sidedress; Sp-split

*Number of years that each N component is lower or higher out of the 30 years of weather simulated for the respective change in fertilizer management.

Table 5.S8 Simulated average change in N loss, maximum and minimum change in any given year, and number of years losses are reduced or increased between selected management scenarios over 30 years of climate variability for the clay loam soil at Woodslee (all results in kg N ha^{-1})

		Injected					**Incorporated**					**Broadcast**				
		Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N
FO to SO	Average	-12.62	0.11	0.32	0.30	-11.89	-5.79	-4.66	0.94	0.10	-9.41	-6.85	-11.30	22.97	-0.76	4.05
	Minimum	-25.56	0.00	0.08	-1.65	-24.20	-14.67	-25.79	0.18	-6.63	-32.94	-23.62	-60.97	-14.09	-7.75	-45.73
	Maximum	-2.52	0.46	0.66	2.14	-1.95	-0.30	0.62	3.29	4.68	0.81	3.43	0.03	71.44	2.60	40.20
	Lower loss*	30	0	0	11	30	30	27	0	14	28	28	29	1	20	10
	Higher loss*	0	28	30	19	0	0	3	30	16	2	2	1	29	10	20
SO to SM	Average	0.18	-0.10	-0.44	-0.85	-1.21	-0.79	-0.82	1.18	-1.21	-1.63	0.76	-0.37	-1.65	-0.53	-1.78
	Minimum	-2.93	-0.31	-0.76	-2.24	-5.60	-3.02	-1.73	-4.09	-6.21	-12.09	-4.57	-1.54	-49.72	-3.51	-49.84
	Maximum	2.47	-0.01	-0.16	0.14	0.58	0.65	-0.48	5.12	0.37	2.10	14.71	0.35	41.20	0.87	35.40
	Lower loss	16	30	30	29	28	24	30	9	29	21	12	27	14	19	12
	Higher loss	14	0	0	1	2	6	0	21	1	9	18	3	16	11	18
SM to SdM	Average	0.02	0.00	0.00	0.25	0.28	-0.40	0.00	0.01	0.31	-0.08	-2.36	-0.39	-11.43	-0.17	-14.36
	Minimum	-1.72	0.00	0.00	-1.02	-2.02	-2.18	-0.01	-5.68	-1.51	-5.86	-9.55	-1.20	-81.97	-2.14	-82.42
	Maximum	2.31	0.07	0.00	2.10	2.18	1.91	0.03	5.93	2.16	6.22	0.97	0.93	36.28	1.44	28.05
	Lower loss	14	0	0	13	13	21	1	13	10	15	25	23	19	19	22
	Higher loss	16	3	0	16	17	9	5	15	20	15	5	6	11	11	8
SM to SpM	Average	-0.01	0.00	0.00	0.15	0.14	0.12	0.00	-2.25	0.21	-1.92	-0.44	-0.18	-16.56	-0.05	-17.24
	Minimum	-0.94	0.00	0.00	-0.65	-1.20	-0.96	0.00	-6.65	-0.90	-5.81	-8.90	-0.82	-55.80	-1.15	-56.00
	Maximum	1.64	0.04	0.00	1.35	1.50	1.91	0.04	1.93	1.41	2.26	2.90	0.91	15.23	1.15	11.57
	Lower loss	17	0	0	13	13	14	0	21	9	23	17	22	26	17	26
	Higher loss	13	2	0	16	17	15	7	1	21	7	12	8	4	13	4
SO to SpO	Average	-1.45	0.01	0.95	-0.03	-0.52	-2.05	-0.20	1.25	0.36	-0.64	3.25	0.01	7.68	1.36	12.30
	Minimum	-2.59	-0.01	0.53	-1.26	-2.06	-4.02	-0.49	-0.24	-0.70	-2.93	-0.27	-0.38	-13.18	0.61	-6.63
	Maximum	-0.33	0.01	1.70	1.20	1.25	-0.78	-0.02	2.87	1.31	2.20	11.93	0.70	28.93	2.35	31.07
	Lower loss	30	1	0	15	22	30	30	1	6	20	1	15	6	0	4
	Higher loss	0	16	30	15	8	0	0	29	24	10	29	15	24	30	26
Application method		**ISM to iSM**					**BSM to iSM**					**BSM to ISM**				
	Average	0.48	0.00	-2.55	-0.59	-2.66	3.02	-1.09	-42.75	-0.56	-41.38	2.53	-1.09	-40.19	0.03	-38.72
	Minimum	-0.42	-0.04	-6.65	-1.64	-6.23	-2.63	-1.90	-98.07	-1.78	-87.19	-2.75	-1.90	-91.96	-0.85	-81.66
	Maximum	2.22	0.03	0.00	-0.17	0.20	11.94	-0.11	-1.59	0.79	-5.09	10.33	-0.14	-1.59	2.22	-4.52
	Lower loss	10	1	21	30	29	2	30	30	22	30	3	30	30	19	30
	Higher loss	20	2	0	0	1	28	0	0	7	0	27	0	0	11	0

i-injected; I-incorporated; B-broadcast; M-mineral; O-organic; S-spring; F-fall; Sd-sidedress; Sp-split

*Number of years that each N component is lower or higher out of the 30 years of weather simulated for the respective change in fertilizer management.

Table 5.S9 Simulated average change in N loss, maximum and minimum change in any given year, and number of years losses are reduced or increased between selected management scenarios over 30 years of climate variability for the sandy loam soil at Woodslee (all results in kg N ha^{-1})

		Injected					**Incorporated**					**Broadcast**				
		Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N
FO to SO	Average	-27.69	0.40	1.88	-0.62	-26.03	-22.67	-3.94	6.41	-1.08	-21.27	-23.25	-7.28	36.77	-1.37	4.86
	Minimum	-64.82	0.01	0.52	-2.40	-63.63	-54.35	-24.44	0.99	-7.89	-46.06	-49.19	-31.70	11.83	-8.26	-21.84
	Maximum	-8.44	1.38	3.96	1.32	-5.17	-6.67	0.28	19.13	2.57	-4.00	-7.68	0.00	80.10	1.61	53.14
	Lower loss*	30	0	0	23	30	30	28	0	25	30	30	29	0	29	11
	Higher loss*	0	30	30	7	0	0	2	30	5	0	0	0	30	1	19
SO to SM	Average	-4.55	-0.46	-2.02	-0.42	-7.45	-3.14	-0.27	-2.23	-0.40	-6.04	-1.81	-0.07	-21.82	-0.20	-23.90
	Minimum	-10.06	-1.36	-3.54	-2.13	-11.66	-6.71	-1.13	-16.65	-3.84	-18.56	-6.20	-0.84	-63.73	-3.23	-69.02
	Maximum	-1.35	-0.03	-0.90	-0.12	-4.55	-0.35	0.08	6.92	0.04	4.85	2.67	0.34	16.71	0.14	10.21
	Lower loss	30	30	30	30	30	30	29	20	29	25	24	19	25	24	26
	Higher loss	0	0	0	0	0	0	1	10	1	5	6	11	5	5	4
SM to SdM	Average	-2.37	0.00	-0.10	0.09	-2.37	-2.97	-0.05	0.73	0.11	-2.18	-4.19	-0.18	9.09	0.10	4.82
	Minimum	-13.71	-0.03	-1.86	-0.10	-13.94	-12.91	-0.24	-12.12	-0.12	-19.86	-13.56	-0.51	-41.34	-0.27	-40.78
	Maximum	0.30	0.13	0.81	0.62	1.04	0.23	0.08	12.82	1.06	10.78	0.44	0.51	51.04	1.23	45.10
	Lower loss	27	11	11	6	27	28	21	11	3	15	29	26	10	6	11
	Higher loss	3	6	8	24	3	2	6	18	25	15	1	4	20	24	19
SM to SpM	Average	-1.60	0.01	-0.24	0.05	-1.78	-1.78	-0.02	-2.62	0.08	-4.34	-2.11	-0.08	-3.07	0.07	-5.18
	Minimum	-8.65	-0.02	-1.86	-0.08	-9.03	-7.62	-0.14	-15.83	-0.06	-17.30	-7.98	-0.31	-37.70	-0.41	-36.91
	Maximum	0.22	0.09	0.00	0.31	0.32	0.45	0.06	5.76	0.73	4.64	0.68	0.29	23.34	1.00	19.77
	Lower loss	25	9	13	7	27	27	20	17	5	23	29	23	16	6	18
	Higher loss	4	10	0	22	3	3	9	10	24	7	1	6	14	23	12
SO to SpO	Average	-2.26	0.00	1.81	0.17	-0.27	-2.89	-0.11	0.34	0.29	-2.37	0.76	0.04	4.53	0.33	5.66
	Minimum	-10.39	-0.04	-0.53	-0.05	-8.58	-9.53	-0.37	-4.25	0.02	-12.09	-1.87	-0.25	-18.04	-0.04	-14.93
	Maximum	-0.29	0.02	2.98	0.35	1.77	-0.38	0.01	5.66	0.65	1.64	4.32	0.33	27.53	0.66	29.58
	Lower loss	30	8	1	3	12	30	29	15	0	23	10	11	6	1	6
	Higher loss	0	9	29	27	18	0	1	15	30	7	20	18	24	29	24
Application method		**ISM to iSM**					**BSM to iSM**					**BSM to ISM**				
	Average	-0.42	-0.32	-5.20	-0.09	-6.03	-0.07	-0.70	-49.62	-0.13	-50.52	0.35	-0.38	-44.43	-0.03	-44.49
	Minimum	-1.28	-0.50	-16.55	-0.19	-17.07	-3.59	-1.12	-98.70	-0.25	-98.93	-2.71	-0.68	-85.41	-0.12	-84.92
	Maximum	0.44	-0.07	0.00	0.10	-0.80	3.75	-0.28	-1.93	0.19	-5.97	3.87	-0.11	-1.93	0.09	-4.87
	Lower loss	23	30	20	28	30	16	30	30	29	30	12	30	30	22	30
	Higher loss	7	0	0	2	0	14	0	0	1	0	18	0	0	5	0

i-injected; I-incorporated; B-broadcast; M-mineral; O-organic; S-spring; F-fall; Sd-sidedress; Sp-split

*Number of years that each N component is lower or higher out of the 30 years of weather simulated for the respective change in fertilizer management.

Table 5.S10 Simulated average change in N loss, maximum and minimum change in any given year, and number of years losses are reduced or increased between selected management scenarios over 30 years of climate variability for the sandy loam soil at Gilmore City (results in kg N ha^{-1})

		Injected					Incorporated					Broadcast				
		Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N	Leach N	Runoff N	NH_3	N_2O	Reactive N
FO to SO	Average	-16.70	0.03	4.30	-2.53	-14.90	-16.13	-2.30	11.49	-3.56	-10.50	-23.08	-3.55	46.66	-4.46	15.57
	Minimum	-31.10	-0.08	0.41	-4.24	-28.46	-31.98	-4.57	-0.04	-6.49	-28.59	-43.02	-6.39	15.51	-9.54	-23.43
	Maximum	-4.75	0.12	8.68	-0.99	-1.08	-5.43	-1.33	28.75	-1.36	10.47	-8.61	-1.40	73.33	-1.75	47.15
	Lower loss*	30	9	0	30	30	30	30	1	30	25	30	30	0	30	6
	Higher loss*	0	21	30	0	0	0	0	29	0	5	0	0	30	0	24
SO to SM	Average	-0.94	-0.09	-4.34	-0.47	-5.85	-0.12	-0.02	-5.55	-0.16	-5.85	1.34	0.01	-17.47	0.01	-16.11
	Minimum	-2.72	-0.16	-8.73	-0.70	-9.97	-2.47	-0.06	-30.18	-0.43	-28.63	-2.84	-0.04	-36.54	-0.26	-34.13
	Maximum	0.40	-0.02	-1.20	-0.19	-2.05	2.79	0.08	10.40	0.34	10.04	10.31	0.19	12.80	0.73	12.04
	Lower loss	27	30	30	30	30	17	21	23	26	24	10	18	28	17	28
	Higher loss	3	0	0	0	0	13	5	7	3	6	20	9	2	11	2
SM to SdM	Average	-2.82	0.02	-0.14	0.10	-2.85	-3.38	0.01	-1.40	0.07	-4.70	-1.70	-0.02	-0.87	0.01	-2.58
	Minimum	-6.66	0.00	-2.39	-0.07	-6.59	-8.41	-0.02	-17.05	-0.07	-22.51	-4.79	-0.13	-60.84	-0.47	-63.22
	Maximum	-0.48	0.17	0.60	0.33	-0.33	-0.57	0.13	10.96	0.33	5.71	1.26	0.03	39.18	0.33	35.70
	Lower loss	30	0	9	2	30	30	15	17	4	21	28	23	14	10	14
	Higher loss	0	13	7	27	0	0	10	13	25	9	2	3	16	18	16
SM to SpM	Average	-1.80	0.01	-0.23	0.05	-1.96	-2.01	0.01	-4.41	0.06	-6.35	-0.08	0.00	-10.69	0.04	-10.74
	Minimum	-4.53	0.00	-1.09	-0.05	-4.46	-5.82	-0.01	-19.77	-0.07	-20.91	-1.45	-0.12	-46.78	-0.42	-48.22
	Maximum	-0.31	0.08	0.00	0.20	-0.29	-0.42	0.11	6.74	0.22	3.76	3.31	0.06	21.40	0.46	19.55
	Lower loss	30	0	11	5	30	30	8	19	3	25	17	15	23	7	25
	Higher loss	0	9	0	25	0	0	9	9	26	5	13	8	7	23	5
SO to SpO	Average	-1.80	0.00	1.76	0.15	0.11	-2.31	0.00	1.94	0.19	-0.18	3.24	0.01	4.49	0.30	8.04
	Minimum	-5.31	-0.02	0.21	-0.07	-2.86	-5.66	-0.04	-9.98	-0.11	-11.93	-0.05	-0.01	-14.20	0.01	-8.93
	Maximum	-0.01	0.01	3.21	0.62	2.55	-0.09	0.01	21.06	0.76	18.35	7.83	0.10	21.53	0.94	23.77
	Lower loss	30	7	0	3	15	30	15	15	4	18	1	3	9	0	7
	Higher loss	0	8	30	27	15	0	7	15	26	12	29	15	21	30	23
Application method		ISM to iSM					BSM to iSM					BSM to ISM				
	Average	-0.49	-0.02	-7.35	-0.05	-7.92	3.09	-0.03	-61.96	-0.03	-58.92	3.59	-0.01	-54.61	0.03	-51.01
	Minimum	-1.75	-0.04	-19.40	-0.18	-18.25	-0.92	-0.09	-97.36	-0.25	-93.93	-0.56	-0.05	-81.79	-0.13	-78.46
	Maximum	1.51	0.05	0.00	0.22	-0.61	9.82	0.16	-29.34	0.60	-27.64	8.48	0.12	-29.34	0.46	-26.24
	Lower loss	26	24	23	24	30	1	25	30	22	30	1	23	30	18	30
	Higher loss	4	4	0	6	0	29	5	0	8	0	29	7	0	10	0

i-injected; I-incorporated; B-broadcast; M-mineral; O-organic; S-spring; F-fall; Sd-sidedress; Sp-split

*Number of years that each N component is lower or higher out of the 30 years of weather simulated for the respective change in fertilizer management

Table 5.S11 Average predicted reactive N loss over 30 years at the Alfred location

Treat-ment	Soil	N_2O (kg N ha^{-1})		NH_3 (kg N ha^{-1})		N Leach (kg N ha^{-1})		N Runoff (kg N ha^{-1})		Silage (kg DM ha^{-1})		Reactive N loss (kg N ha^{-1})	Reactive N (kg) per ton dry silage
iSM	C	2.9	e*	0.0	e	13.7	cde	0.3	de	15769	a	16.9	1.07
iSpM	C	3.2	de	0.0	e	13.5	cde	0.3	de	15776	a	17.0	1.08
iSdM	C	3.3	cde	0.0	e	13.4	cde	0.3	de	15777	a	17.1	1.08
iSO	C	3.3	de	0.2	e	12.7	de	0.3	de	15386	a	16.5	1.07
iSpO	C	3.6	cde	0.5	e	12.3	de	0.3	de	15293	a	16.7	1.09
iFO	C	3.5	cde	0.1	e	18.0	ab	0.3	e	15209	a	21.9	1.44
ISM	C	3.4	cde	1.3	e	13.6	cde	0.3	de	15706	a	18.6	1.19
ISpM	C	3.3	cde	0.0	e	13.4	cde	0.3	de	15747	a	17.0	1.08
ISdM	C	3.5	cde	0.2	e	13.3	cde	0.3	de	15735	a	17.3	1.10
ISO	C	4.0	bc	0.4	e	13.1	de	0.6	cde	15239	a	18.1	1.18
ISpO	C	4.3	ab	0.9	e	12.4	de	0.5	cde	15108	a	18.2	1.20
IFO	C	4.5	ab	0.4	e	17.5	b	3.3	b	14937	a	25.7	1.72
BSM	C	3.9	bcd	25.4	b	13.5	cde	1.0	cde	15805	a	43.7	2.77
BSpM	C	4.3	ab	19.3	c	14.1	bc	1.0	cde	15963	a	38.7	2.43
BSdM	C	4.3	ab	30.6	a	12.8	de	0.9	cde	15819	a	48.7	3.08
BSO	C	3.8	bcd	24.2	b	11.9	e	1.1	cd	14965	a	41.0	2.74
BSpO	C	5.0	a	28.3	a	15.2	c	1.2	c	15933	a	49.7	3.12
BFO	C	4.9	a	15.1	d	19.6	a	10.5	a	15377	a	50.2	3.26
iSM	SL	2.2	ef	0.0	e	31.8	c	0.4	c	13413	a	34.4	2.56
iSpM	SL	2.3	ef	0.0	e	31.5	c	0.4	c	13435	a	34.2	2.55
iSdM	SL	2.3	ef	0.1	e	31.3	c	0.4	c	13436	a	34.1	2.54
iSO	SL	2.6	cdef	0.9	e	34.7	c	0.6	c	13437	a	38.8	2.89
iSpO	SL	2.8	bcde	2.5	e	34.1	c	0.6	c	13412	a	40.0	2.98
iFO	SL	3.2	b	0.2	e	67.6	a	0.4	c	9172	b	71.4	7.79
ISM	SL	2.3	ef	1.5	e	32.4	c	0.5	c	13347	a	36.6	2.74
ISpM	SL	2.3	ef	0.1	e	31.7	c	0.4	c	13429	a	34.6	2.57
ISdM	SL	2.4	def	0.7	e	31.4	c	0.4	c	13424	a	35.0	2.60
ISO	SL	2.7	bcdef	2.1	e	33.5	c	0.5	c	13260	a	38.8	2.93
ISpO	SL	3.0	bc	4.1	e	33.0	c	0.5	c	13256	a	40.6	3.06
IFO	SL	3.7	a	1.3	e	61.1	b	4.7	b	9842	b	70.8	7.19
BSM	SL	2.4	def	31.9	c	33.1	c	0.5	c	13347	a	67.9	5.09
BSpM	SL	2.5	edef	26.2	d	32.8	c	0.6	c	13387	a	62.1	4.64
BSdM	SL	2.5	cdef	41.9	b	31.6	c	0.5	c	13248	a	76.5	5.77
BSO	SL	2.6	cdef	44.8	b	33.3	c	0.6	c	12733	a	81.2	6.38
BSpO	SL	2.9	bcd	51.4	a	35.2	c	0.6	c	13527	a	90.2	6.67
BFO	SL	4.0	a	28.0	d	60.2	b	9.4	a	10193	b	101.7	9.97

i-injected; I-incorporated; B-broadcast; M-mineral; O-organic; S-spring; F-fall; Sd-sidedress; Sp-split
*Significant difference between management practices if there are no intersected letter between treatments ($p<0.05$). Analysis of Variance with Duncan test within the same soil type (C or SL).

Table 5.S12 Average predicted reactive N loss over 30 years at the Woodslee location

Treat-ment	Soil	N_2O (kg N ha^{-1})		NH_3 (kg N ha^{-1})		N Leach (kg N ha^{-1})		N Runoff (kg N ha^{-1})		Silage (kg DM ha^{-1})		Reactive N loss (kg N ha^{-1})	Reactive N (kg) per ton dry silage
iSM	CL	7.0	f *	0.0	f	16.8	cde	0.5	c	17532	a	24.2	1.38
iSpM	CL	7.1	ef	0.0	f	16.8	cde	0.5	c	17546	a	24.4	1.39
iSdM	CL	7.2	ef	0.0	f	16.8	cde	0.5	c	17537	a	24.5	1.40
iSO	CL	7.8	cdef	0.4	f	16.6	cde	0.6	c	17584	a	25.4	1.45
iSpO	CL	7.8	def	1.4	f	15.2	de	0.6	c	17638	a	24.9	1.41
iFO	CL	7.5	ef	0.1	f	29.2	a	0.5	c	17555	a	37.3	2.13
ISM	CL	7.5	ef	2.6	f	16.3	cde	0.5	c	17541	a	26.9	1.53
ISpM	CL	7.8	def	0.3	f	16.4	cde	0.5	c	17533	a	25.0	1.42
ISdM	CL	7.9	cdef	2.6	f	15.9	de	0.5	c	17525	a	26.8	1.53
ISO	CL	8.8	abc	1.4	f	17.1	cd	1.3	c	17558	a	28.5	1.62
ISpO	CL	9.1	a	2.6	f	15.0	def	1.1	c	17648	a	27.9	1.58
IFO	CL	8.7	abcd	0.4	f	22.9	b	6.0	b	17217	a	37.9	2.20
BSM	CL	7.5	ef	42.7	b	13.8	def	1.6	c	17334	a	65.6	3.78
BSpM	CL	7.5	ef	26.2	d	13.3	def	1.4	c	17320	a	48.4	2.79
BSdM	CL	7.3	ef	31.3	c	11.4	f	1.2	c	16983	a	51.2	3.02
BSO	CL	8.0	bcde	44.4	b	13.0	ef	1.9	c	17215	a	67.4	3.91
BSpO	CL	9.4	a	52.1	a	16.3	cde	1.9	c	18021	a	79.7	4.42
BFO	CL	8.8	ab	21.4	e	19.9	bc	13.2	a	16851	a	63.3	3.76
iSM	SL	3.4	e	0.2	h	42.3	b	0.6	c	12017	ab	46.5	3.87
iSpM	SL	3.5	de	0.0	h	40.7	b	0.6	c	12576	ab	44.7	3.56
iSdM	SL	3.5	de	0.1	h	39.9	b	0.6	c	12837	a	44.1	3.44
iSO	SL	3.8	cde	2.3	fgh	46.8	b	1.0	c	12162	ab	54.0	4.44
iSpO	SL	4.0	cde	4.1	efgh	44.6	b	1.0	c	12438	ab	53.7	4.32
iFO	SL	4.5	bc	0.4	h	74.5	a	0.6	c	8096	d	80.0	9.88
ISM	SL	3.5	de	5.4	efgh	42.7	b	0.9	c	11726	ab	52.5	4.48
ISpM	SL	3.6	de	2.8	efgh	40.9	b	0.9	c	12430	ab	48.2	3.88
ISdM	SL	3.6	de	6.2	efg	39.7	b	0.9	c	12659	ab	50.4	3.98
ISO	SL	3.9	cde	7.7	ef	45.8	b	1.2	c	11519	b	58.6	5.08
ISpO	SL	4.2	cd	8.0	e	42.9	b	1.1	c	11973	ab	56.2	4.69
IFO	SL	5.0	ab	1.2	gh	68.5	a	5.1	b	7968	d	79.8	10.02
BSM	SL	3.5	de	49.9	c	42.3	b	1.3	c	11547	b	97.0	8.40
BSpM	SL	3.6	de	46.8	c	40.2	b	1.2	c	12099	ab	91.8	7.59
BSdM	SL	3.6	de	59.0	b	38.1	b	1.1	c	12039	ab	101.8	8.46
BSO	SL	3.7	de	71.7	a	44.1	b	1.3	c	10095	c	120.9	11.98
BSpO	SL	4.1	cde	76.2	a	44.9	b	1.4	c	11736	ab	126.6	10.79
BFO	SL	5.1	a	34.9	d	67.4	a	8.6	a	7898	d	116.1	14.70

i-injected; I-incorporated; B-broadcast; M-mineral; O-organic; S-spring; F-fall; Sd-sidedress; Sp-split

*Significant difference between management practices if there are no intersected letter between treatments ($p<0.05$). Analysis of Variance with Duncan test within the same soil type (CL or SL).

Table 5.S13 Average predicted reactive N loss over 30 years at the Gilmore City location

Treat-ment	Soil	N_2O (kg N ha^{-1})		NH_3 (kg N ha^{-1})		N Leach (kg N ha^{-1})		N Runoff (kg N ha^{-1})		Silage (kg DM ha^{-1})		Reactive N loss (kg N ha^{-1})	Reactive N (kg) per ton dry silage
iSM	CL	4.2	def *	0.1	f	26.3	b	0.1	c	16963	a	30.7	1.81
iSpM	CL	4.4	def	0.0	f	24.7	bcd	0.1	c	16988	a	29.2	1.72
iSdM	CL	4.5	de	0.1	f	23.8	bcde	0.1	c	16996	a	28.5	1.68
iSO	CL	4.5	de	0.7	f	25.9	bc	0.1	c	16917	a	31.2	1.84
iSpO	CL	4.6	d	2.0	f	24.3	bcd	0.1	c	16912	a	31.0	1.83
iFO	CL	5.9	c	0.1	f	39.3	a	0.1	c	16658	ab	45.4	2.72
ISM	CL	4.1	defg	4.2	f	26.0	bc	0.1	c	16952	a	34.4	2.03
ISpM	CL	4.2	def	0.5	f	24.9	bcd	0.1	c	16988	a	29.7	1.75
ISdM	CL	4.3	def	3.3	f	23.7	bcde	0.1	c	16978	a	31.3	1.85
ISO	CL	3.8	fg	2.2	f	25.7	bc	0.1	c	16818	a	31.8	1.89
ISpO	CL	4.0	defg	5.2	f	23.7	bcde	0.1	c	16833	a	33.0	1.96
IFO	CL	6.7	b	0.8	f	37.7	a	2.4	b	16410	ab	47.6	2.90
BSM	CL	3.5	g	52.7	b	18.4	ef	0.1	c	15247	b	74.7	4.90
BSpM	CL	3.5	g	35.7	d	19.7	def	0.1	c	16227	ab	58.9	3.63
BSdM	CL	3.5	g	42.9	c	16.9	f	0.1	c	15554	ab	63.4	4.08
BSO	CL	3.6	g	56.8	b	20.2	cdef	0.1	c	15232	b	80.7	5.30
BSpO	CL	3.9	efg	64.8	a	24.0	bcde	0.1	c	16935	a	92.9	5.49
BFO	CL	7.5	a	22.2	e	41.0	a	4.2	a	16549	ab	74.7	4.52
iSM	SL	2.1	e	0.4	h	43.1	b	0.1	c	14482	ab	45.7	3.16
iSpM	SL	2.2	e	0.2	h	41.3	b	0.1	c	14571	a	43.8	3.00
iSdM	SL	2.2	de	0.3	h	40.2	b	0.1	c	14606	a	42.9	2.94
iSO	SL	2.6	de	4.8	efg	44.0	b	0.2	c	14549	a	51.6	3.55
iSpO	SL	2.8	d	6.5	fg	42.2	b	0.2	c	14544	a	51.7	3.55
iFO	SL	5.2	c	0.5	h	60.7	a	0.2	c	13911	abc	66.5	4.78
ISM	SL	2.2	e	7.8	f	43.5	b	0.1	c	14338	abc	53.6	3.74
ISpM	SL	2.3	de	3.4	efg	41.5	b	0.1	c	14530	a	47.3	3.25
ISdM	SL	2.3	de	6.4	fg	40.2	b	0.1	c	14550	a	48.9	3.36
ISO	SL	2.4	de	13.3	e	43.7	b	0.2	c	13868	abc	59.5	4.29
ISpO	SL	2.6	de	15.3	e	41.4	b	0.1	c	13969	abc	59.3	4.25
IFO	SL	5.9	b	1.8	fg	59.8	a	2.4	b	13385	abc	70.0	5.23
BSM	SL	2.2	e	62.4	b	40.0	b	0.1	c	13082	c	104.7	8.00
BSpM	SL	2.2	e	51.7	c	39.9	b	0.1	c	14245	abc	93.9	6.59
BSdM	SL	2.2	e	61.5	b	38.3	b	0.1	c	14029	abc	102.1	7.28
BSO	SL	2.2	e	79.8	a	38.6	b	0.1	c	11077	d	120.8	10.90
BSpO	SL	2.5	de	84.3	a	41.9	b	0.2	c	13403	abc	128.8	9.61
BFO	SL	6.6	a	33.2	d	61.7	a	3.7	a	13220	bc	105.2	7.96

i-injected; I-incorporated; B-broadcast; M-mineral; O-organic; S-spring; F-fall; Sd-sidedress; Sp-split
*Significant difference between management practices if there are no intersected letter between treatments ($p<0.05$). Analysis of Variance with Duncan test within the same soil type (CL or SL).

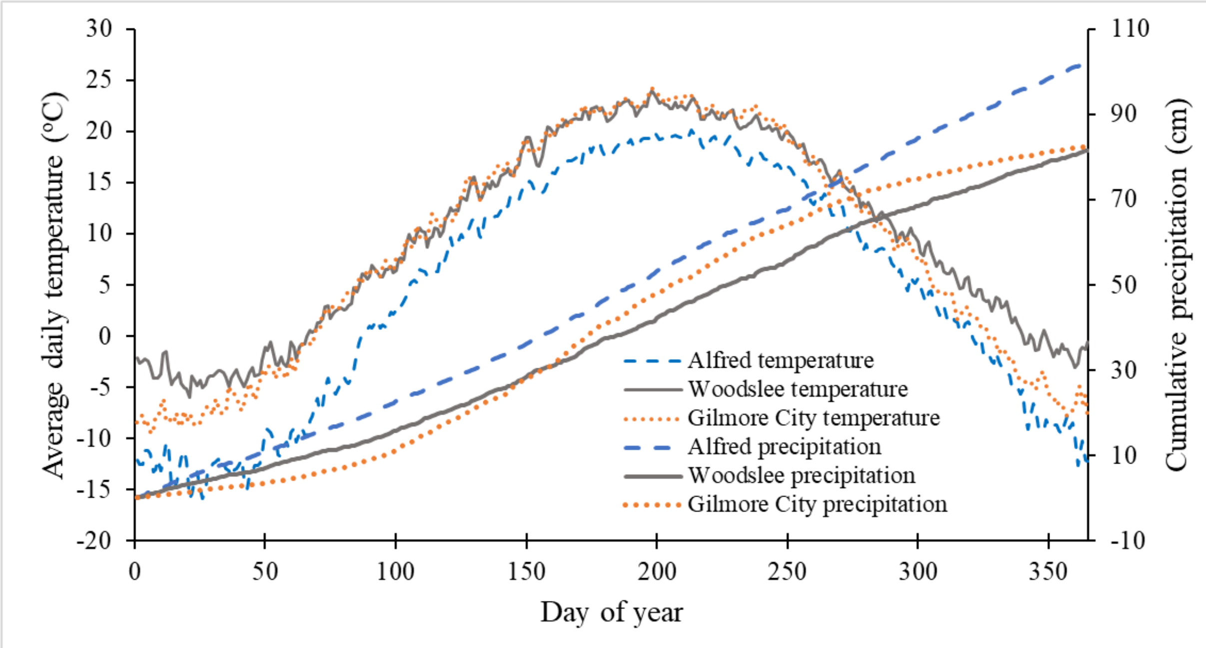

Figure 5.S1. Average daily temperature and cumulative precipitation for the 30 weather years simulated at Alfred, Woodslee and Gilmore City locations

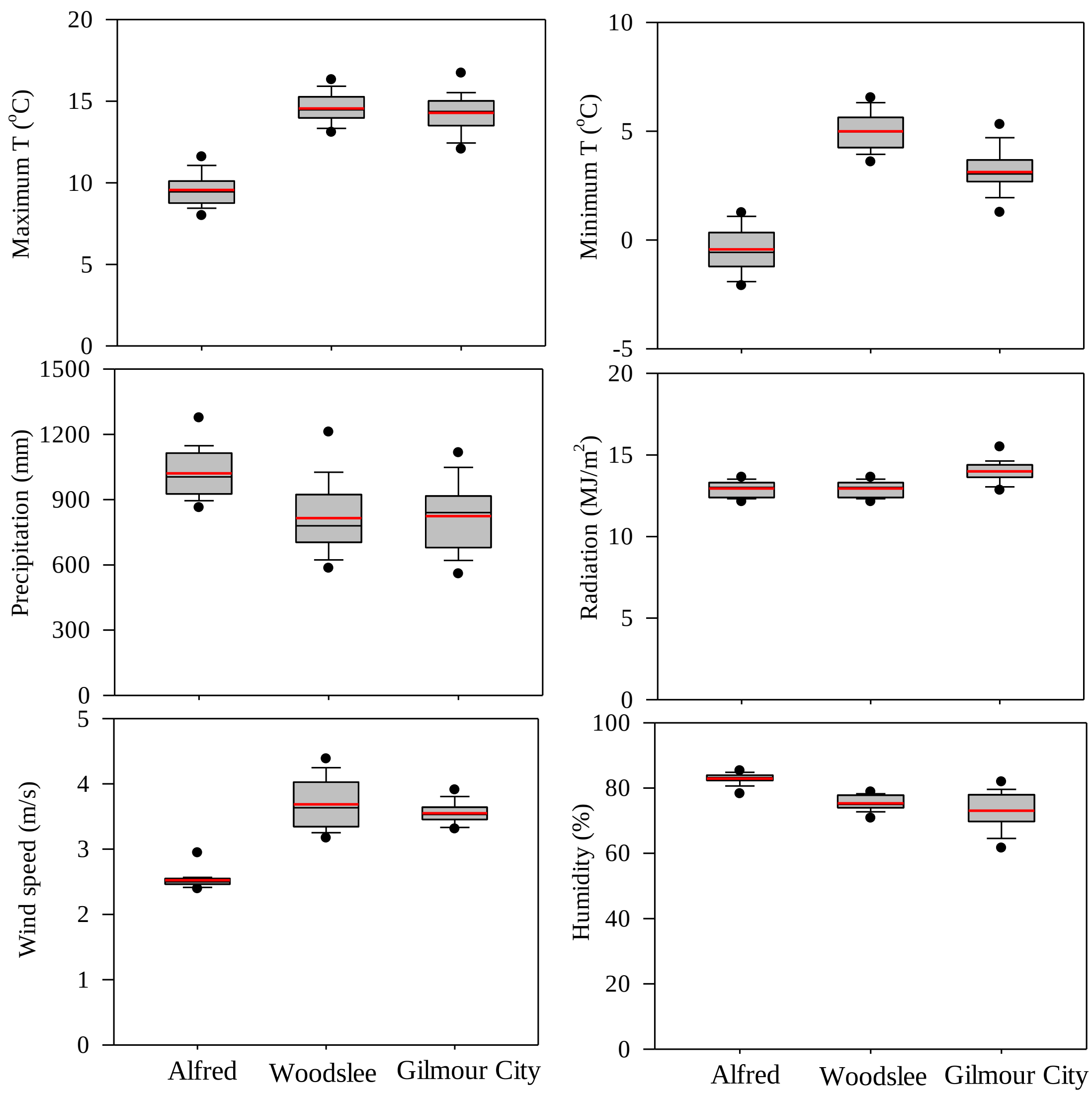

Figure 5.S2 Boxplots showing 30 year range of average annual minimum and maximum temperature (T), precipitation, radiation, wind speed and relative Humidity at Alfred, Woodslee and Gilmore City. The black and red lines, lower and upper edges of the boxes, and bars and dots in outside the boxes represent median and mean values, 25th and 75th, 5th and 95th, and <5th and >95th percentiles of all data, respectively.

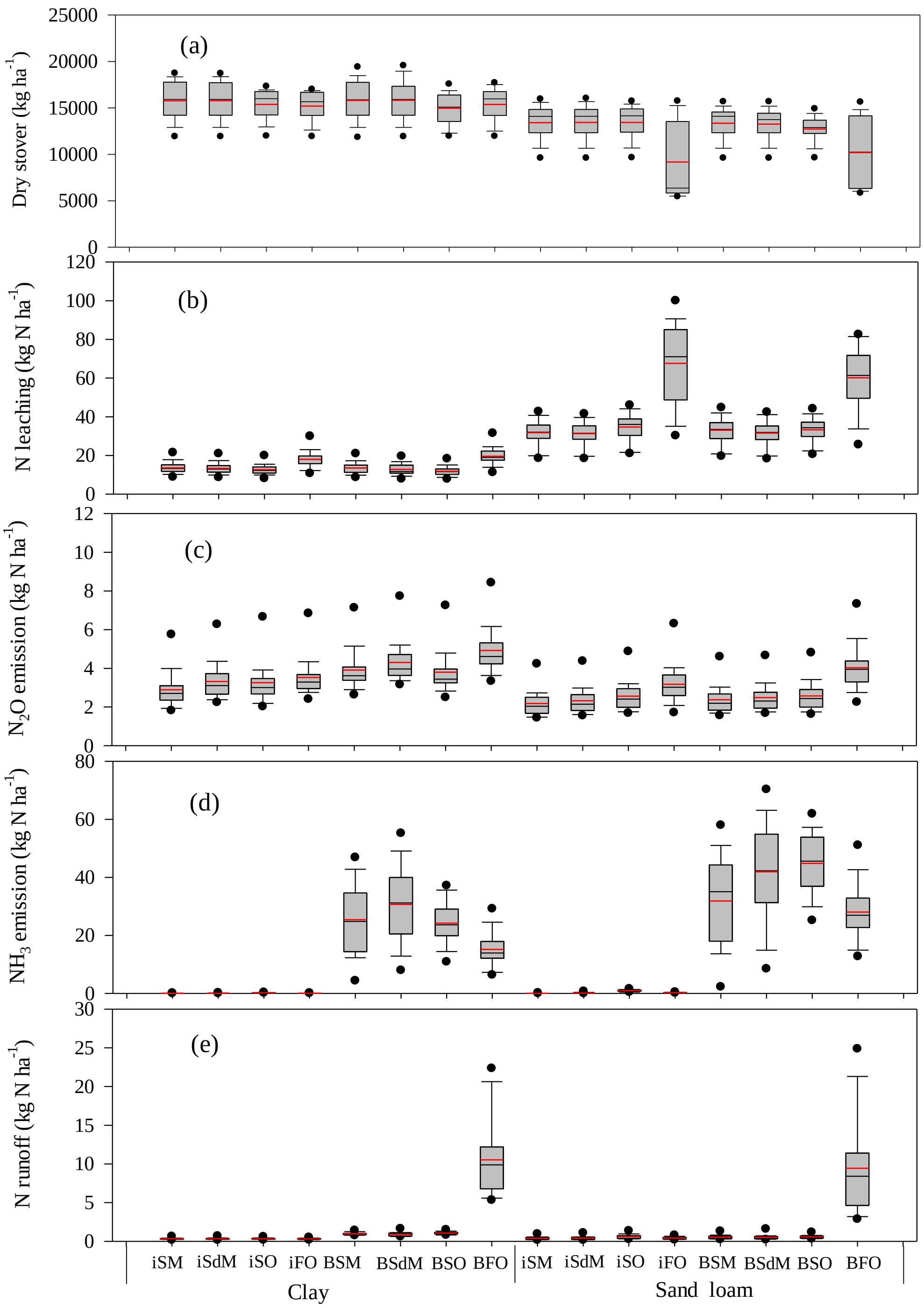

Figure 5.S3. Boxplots showing impacts of selected fertilizer management across 30 years of climate variability at the Alfred location on a) dry silage biomass b) N leaching to tiles, c) N_2O emissions, d) NH_3 volatilization, and e) N runoff. The black and red lines, lower and upper edges of the boxes, and bars and dots in outside the boxes represent median and mean values, 25th and 75th, 5th and 95th, and <5th and >95th percentiles of all data, respectively.

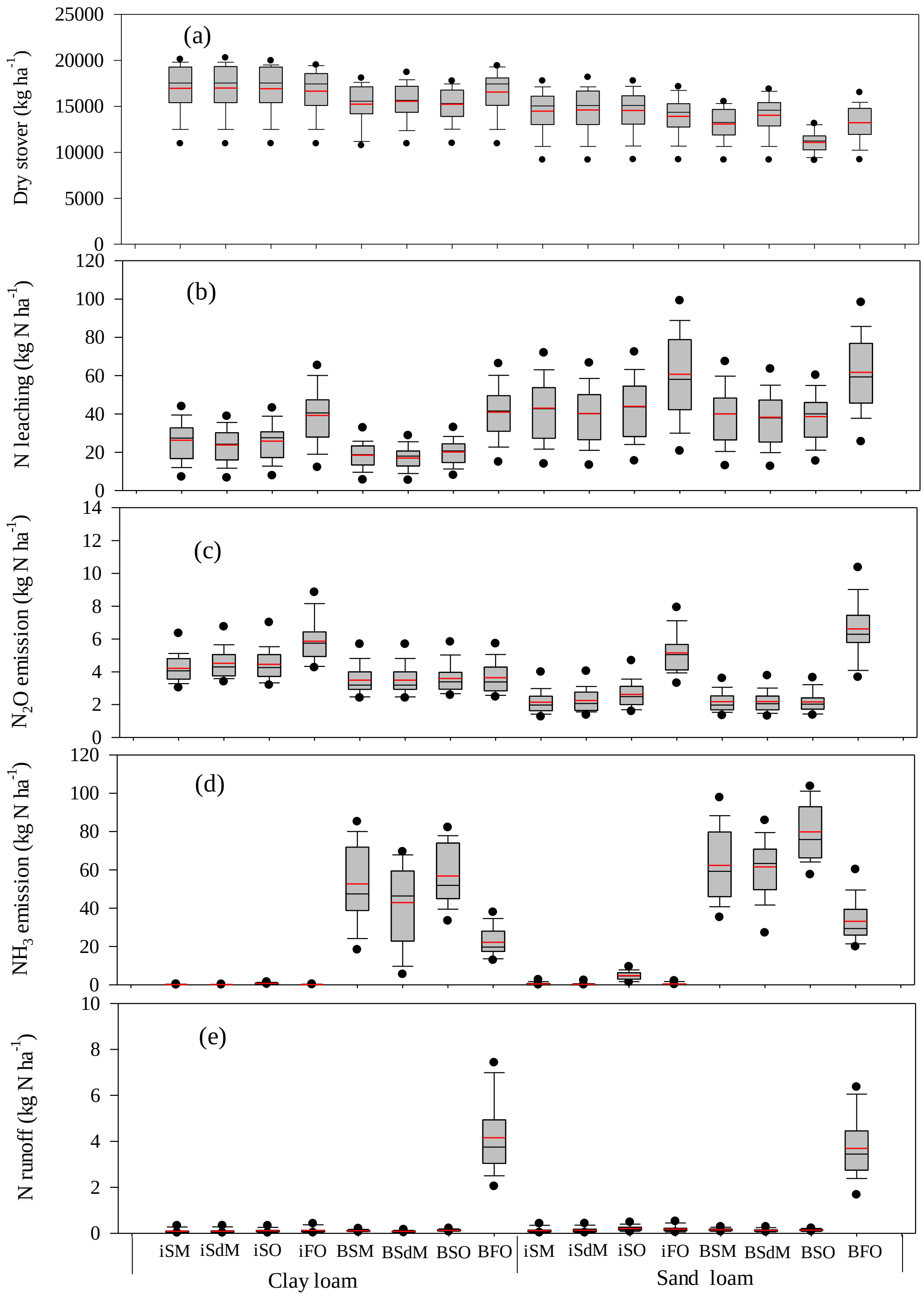

Figure 5.S4. Boxplots showing impacts of selected fertilizer management across 30 years of climate variability at the Gilmore City location on a) dry silage biomass b) N leaching to tiles, c) N_2O emissions, d) NH_3 volatilization, and e) N runoff. The black and red lines, lower and upper edges of the boxes, and bars and dots in outside the boxes represent median and mean values, 25th and 75th, 5th and 95th, and <5th and >95th percentiles of all data, respectively.

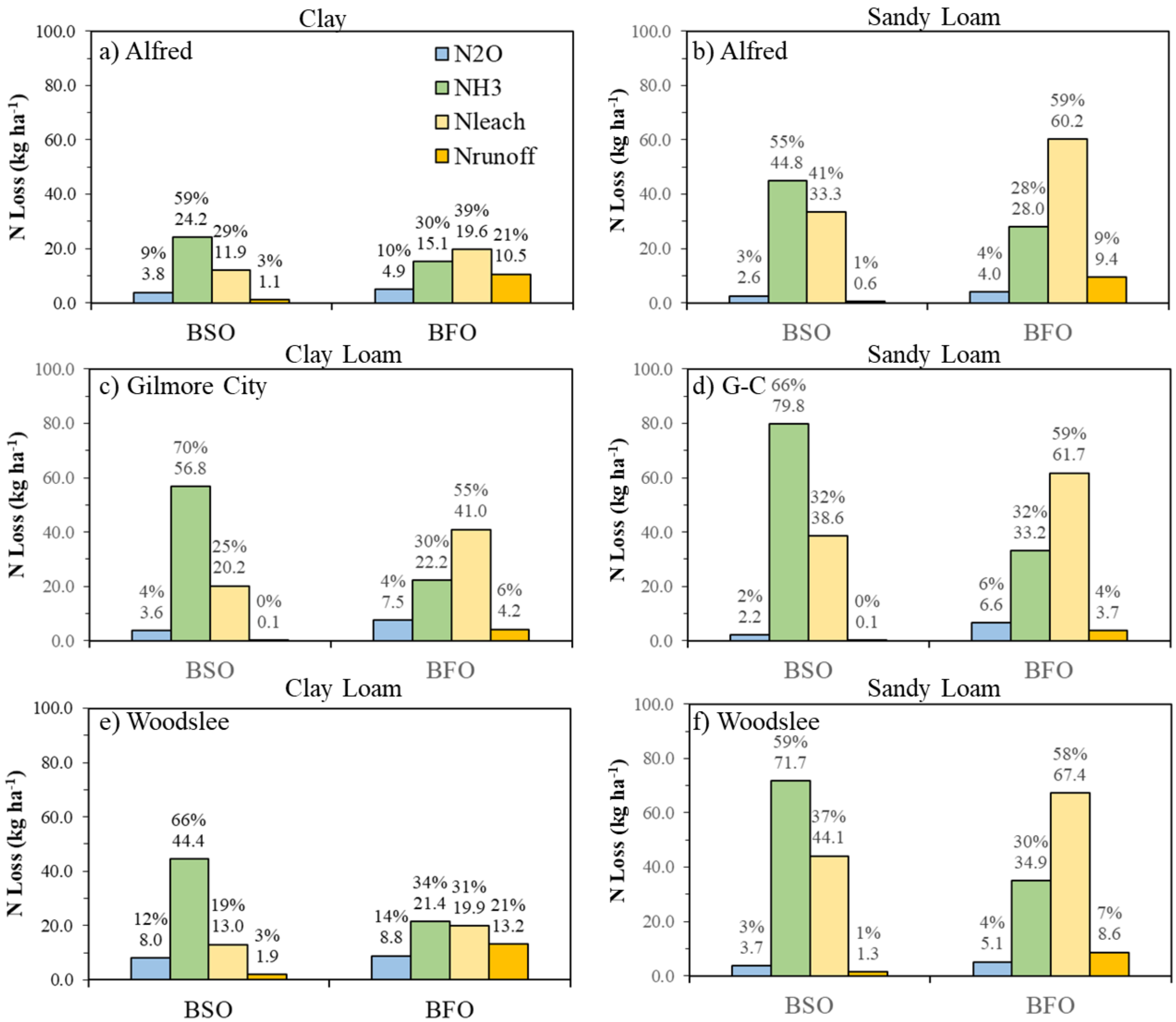

Figure 5.S5. Reactive N loss (N_2O emissions, NH_3 volatilization, N leaching, N runoff) for broadcast spring and fall applied dairy manure slurry for a) clay at Alfred, b) sandy loam at Alfred, c) clay loam at Gilmore City, d) sandy loam at Gilmore City, e) clay loam at Woodslee, and f) sandy loam at Woodslee. BSO refers to broadcast spring applied dairy slurry (organic) and BFO refers to broadcast fall applied dairy slurry (organic).

Connecting text to Chapter 6

In Chapter 5 an assessment of fertilizer management impacts on N losses from cropping systems under long-term climate variability was explored, however, the impacts of possible changes in future climate were not considered. Well developed and calibrated biophysical models can be particularly valuable for simulating climate change impacts, however, there are many alternative modelling approaches used in literature for simulating such impacts which can produce greatly different results. Some of these studies employ simple methods due to limitations in models or due to complications in simulating changes in agronomic practices over time. Thus in Chapter 6 focus is placed on using the revised model presented in Chapter 4, which was enhanced for simulating more accurate hydrology and a larger array of possible management interactions, to explore approaches for simulating climate change impacts on cropping systems and to recommend a plausible approach. The assessments were performed at locations where the model had previously been validated in Chapters 4 and 5, but also at a semi-arid location, Swift Current, to assess modelling approaches in a cool dry region. Additional model validation was performed at this location using long-term crops yields, soil carbon and soil water observations.

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Chapter 6

Towards an approach for modelling the impacts of climate change on cropping systems

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Abstract

Climate change is expected to impact crop growth, reactive nitrogen losses, and soil carbon dynamics in cropping systems worldwide. It is important to develop plausible modelling approaches for predicting the feedbacks of water and nutrient cycling on these outcomes, while incorporating likely changes in agricultural management under a changing climate. We performed case studies at three locations in Canada to explore the impact of modelling approaches that are commonly employed in literature which may adversely impact the simulation of crop yields, soil organic carbon change and N losses. These include the use of a minimum set of weather variables, re-initializing soil status annually, fixed fertilizer application rates, fixed planting dates, and ignoring changes in crop cultivars and rotational impacts. The approaches were compared to a comprehensive base approach where detailed climate drivers, adjustment of planting dates, fertilizer rates based on crop needs, and continuous simulation of soil C&N and water feedbacks were considered. We found that there were significant impacts of all approaches under certain conditions. At the semi-arid location the simulation of crop yields was significantly impacted through changes in evapotranspiration, differences in feedbacks from C&N cycling and under fertilization in the case of the fixed fertilizer approach. Crop yields were strongly impacted by rotational effects at the humid locations. Every modeling approach considered resulted in significant differences in N losses relative to the base approach, either N_2O, N leaching, N runoff or a combination. We conclude that there are often large differences between approaches used for modeling climate change impacts and we recommend that modellers improve their capabilities of simulating expected changes in agronomy and biophysical processes that enable long-term simulation of soil-plant C&N cycling and hydrological feedbacks. This is needed to enable plausible projections of climate change impacts on cropping systems.

6.1 Introduction

Food production using sustainable practices to maintain or increase crop yields while limiting negative anthropogenic influences on the environment is an important global research activity. In most regions of the world it is likely that climate change will strongly influence crop growth and development, soil health, greenhouse gas (GHG) emissions and nutrient losses. In northern latitudes such as in northeast China and the UK some studies have found positive impacts on crop yields (Supit *et al.,* 2010; Chen *et al.,* 2010). A strong influence of climate change is expected in Canada where temperatures are increasing at a rate faster than the global average (Qian *et al.,* 2019: Bush and Lemmen, 2019) and the estimated frost free period for crop growth has increased by approximately 3 weeks since the early twentieth century (Qian *et al.,* 2012). However, in warmer regions globally crop growth may suffer under warmer temperatures. For instance, it was estimated that wheat and maize yields may already be declining, especially in tropical regions, with an estimated global average reduction of 5.5 and 3.8%, respectively (Lobell *et al.,* 2011).

Reactive N losses from currently established cropping systems are generally projected to increase under future warmer climates, including nitrous oxide (N_2O) emissions (Abalos *et al.,* 2016a: Smith *et al.,* 2013: Tian *et al.,* 2012), NO_3^- leaching and runoff (Wang *et al.,* 2015) and ammonia (NH_3) volatilization (Suddick *et al.*, 2012). To reach the increasing demands for food and fibre there will likely be increased N inputs in the future (Snyder *et al.,* 2014) through expansion of agricultural areas and increased intensity, potentially further increasing N losses. Statistical models are useful for estimating changes in yields and sometimes nutrient losses under current climate and management, however, they are not well suited for estimating the feedbacks from soil C&N cycling nor the complex physiological climate impacts on crop growth and development (Basso *et al.,* 2015). The physiological effects of climate on crop growth need to be considered including the impacts of CO_2 fertilization on photosynthesis, water and N use efficiency, temperature and water stress during critical growth phases such as anthesis, and in the case of cool climates frost damage and winterkill (Smith *et al.,* 2013). In order to simulate the impacts of changing stresses on crop production and nutrient losses it is important to include system feedbacks from water, C and N cycling thus a model needs to include robust hydrological and biogeochemical processes and be capable of simulating a wide range of agricultural management. When cool weather cropping systems are considered the impacts of snow cover and soil freeze-thaw dynamics are crucial (Cui and Wang, 2019; Dutta *et al.,* 2018) for determining losses of water and nutrient to runoff and drainage, mechanisms which several prominent crop models currently do not consider. This may be partially why it is common practice in most climate change studies to re-initialize the soil status (water, soil organic carbon [SOC], nutrients) in models each year prior to the growing season (Basso *et al.*, 2015) to avoid the issue. However, the soil status can greatly change over time resulting in significant feedbacks on crop growth (Basso *et al.*, 2015) and environmental outcomes. Higher rates of N leaching and runoff often occur in the non-growing season when there is no crop water and N uptake (Smith *et al.,* 2019c: Gamble *et al.,* 2018: Schwager *et al.,* 2016). Likewise, N_2O emissions are highly influenced by soil water status and can be strongly driven by off-season soil freeze-thaw activity in cool weather systems (Wagner-Riddle *et al.,* 2008). Certain agroecosystem models such as DayCent (del Grosso *et al.*, 2001), the Root Zone Water Quality Model (RZWQM2; Ma *et al.*, 2012) which has DSSAT imbedded and the DeNitrification DeComposition model (DNDC; Li *et al.*, 2012) are capable of dynamically simulating many interdependent soil-plant processes and include over-winter soil freeze-thaw and snow dynamics. The DNDC model is well known for simulating GHG emissions, but over the years it has been expanded for simulating plant growth (Zhang and Niu, 2016), soil C&N cycling, ammonia volatilization and methanogenisis. A Canadian version (DNDCv.CAN) was developed originally to simulate plant-soil-management interactions in cool weather climates (Kroebel *et al.,* 2011) but more recently it was expanded to improve the simulation of several processes (Dutta *et al.*, 2018, 2016a,b; Congreves *et al.*, 2016b; Smith *et al.*, 2013) and to incorporate quasi-2D tile drainage (Smith *et al.*, 2019b).

In addition to the practice of re-initializing models annually there are several other common modelling approaches which need to be investigated for their reliability in representing changes in agricultural systems 1) fixed planting date versus adjustment to accommodate future weather; 2) use of limited weather variables (temperature and precipitation) versus a fuller range or weather inputs; 3) constant fertilizer rates versus changes over time based on crop needs and soil status; 4) monoculture versus crop rotations; and 5) constant crop cultivar versus alternative cultivars to better match changes in seasonal requirements. Simple approaches for modelling management impacts are often employed in many climate change impact studies but it is our hypothesis that these approaches will not successfully account for the changes in soil water and nutrient status under future conditions thus will strongly bias results. The objectives of this study were to i) investigate the implications of using simpler versus more advanced modelling approaches for simulating the impacts of climate change on crop production, SOC change, N_2O emissions and N leaching and runoff; ii) to recommend a viable approach under cool weather climates; and iii) to assess the effect of climate change on crop production and sustainability for common cropping systems in Canada. In doing so we employ the DNDCv.CAN model which was validated using detailed data at three locations, one under a semi-arid climate in western Canada and two under humid conditions in eastern Canada.

6.2 Methodology

6.2.1 Experimental sites

Cropping system datasets from three sites in Canada were used to calibrate and validate DNDC for simulating crop yields, soil carbon, N_2O emissions, nitrate leaching and runoff. Before implementing approaches for modelling climate change impacts it is important to ensure that the model responds reasonably to inter-annual climatic drivers at each location. We purposefully chose sites that differed greatly in precipitation to study a larger range of possible impacts on N loss and SOC change. For instance, at the semi-arid Swift Current site we expected much less N loss through leaching (Campbell *et al.,* 2006) and minimal N_2O emissions (Grant *et al.,* 2016) in comparison to the more humid sites in western Canada. General data availability at each site is noted in Table 6.1 and further site details follow.

Table 6.1 Soil and climate characteristics at Alfred, Woodslee and Swift Current research plots

Location and data collection period	Soil classification	Average annual temp. (°C)	Average annual precip. (mm)	PET⁺ (mm)	Soil characteristics (20 cm)			Data availability			
					Soil texture (%)	SOC (Mg C ha^{-1})	Bulk density (g cm^{-3})	Crop yields	SOC	N_2O	NO_3^- leach
Alfred, Ontario 45.34° N, 74.55° W (2011-2014)	Orthic Humic Gleysol	4.5	1021	944	35 sand 18 silt 47 clay	69.6	1.34	√	x	√	√
Woodslee, Ontario 42°13'N, 82°44'W (1959-2015)	Orthic Humic Gleysol	8.9	831	1046	28 sand 34 silt 38 clay	56.7	1.42	√	√	√	√
Swift Current, Saskatchewan 50°17'N, 107°48'W (1967-2009)	Orthic Brown Chernozem	4.8	359	1153	33 sand 35 silt 32 clay	40.7	1.34	√	√	x	x

⁺ Average potential evapotranspiration as estimated by the Penman Montieth method from 1981-2010

6.2.1.1 Swift Current site

A long-term rotation trial was established at the Swift Current Research Station, Saskatchewan (lat. 50°17’ N, long. 107°48’W) in 1966 to study differences in cropping systems with various levels of fallow, with and without fertilizer N and P in semiarid conditions. Annual precipitation was 359 mm with 212 mm falling in the growing season. In addition to the lowest rainfall at this site it also has high potential evapotranspiration (PET) due to higher wind speeds (Table 6.1). Prior to the study the field had been cropped with fallow-wheat since 1922. In our current study, for model validation, we used the fertilized wheat and wheat-lentil rotations over a long time frame from 1967-2009. The soil is characterized as a Swinton Loam (Ayres *et al.*, 1985) in the Brown Chernozem (Aridic Haploboroll) Great Group (Table 6.1). Fertilizer N was applied each year for wheat as NH_4NO_3 based on soil N testing. A recommended total N rate of 65 kg ha^{-1} (soil N test + fertilizer) was applied on spring wheat from 1967 to 1989 (soil-testing laboratory of the University of Saskatchewan). From 1990 onward a total rate of 90 kg ha^{-1} for spring wheat on fallow and 73 kg ha^{-1} for wheat on stubble was applied (Campbell *et al.*, 2005). Phosphorous was applied as ammonium phosphate at seeding at a rate of 10 kg P ha^{-1}. The timing of seeding and harvest varied from year to year based on weather conditions but seeding was typically in May and harvest in late August. Tillage was minimal in wheat years with a single cultivator pass in the spring. In fallow years multiple passes were made to control weeds. A wide array of measurements were taken at this research station including annual grain yields and periodic measurements of straw yields, grain N, straw N, soil C, soil N, soil moisture and N_2O emissions from 2001 to 2003 and more detailed description sof the site design and management is available in Grant *et al.* (2016), Campbell *et al.* (1983, 2005, 2007) and Campbell and Zentner (1993).

6.2.1.2 Woodslee site

A field study was established in 1959 at the Hon. Eugene F. Whelan Experimental Farm, Woodslee, Ontario (lat. 42.28N, long. 83.08W) to determine the long-term impacts of fertilizer and crop rotation on crop yields, soil health, and N losses. The study was setup on a tile drained Brookston clay loam and the site was relatively warm for Canada with a moderate level of 831mm annual average precipitation (Table 6.1). The cropping systems used for model setup and validation in this study included fertilized continuous corn and a fertilized 4 yr rotation of corn-oats-alfalfa-alfalfa with each phase present each year. Planting typically occurred during May but occasionally extended into late April or early June, depending on weather conditions. Continuous corn, rotational corn and oats were fertilized with starter fertilizer (8-32-16) 16.8 kg N ha^{-1} incorporated into the top 10 cm of soil near the time of planting. Sidedress urea ammonium nitrate (UAN) fertilizer at the rate of 112 kg N ha^{-1} was banded between the corn rows near mid June at the six-leaf stage. Further details regarding the site setup and management is available in Drury *et al.* (1998) and Reynolds *et al.* (2014). To initialize and validate the DNDC model we used measured yield data from 1959-2015, SOC data at various soil depths from 2004-2007, and N_2O was measured using a chamber approach from continuous corn and each phase of the corn-oat-alfalfa-alfalfa rotation. Nitrous oxide was measured 79 times, with 12 replicate, from spring 2010 until fall 2013.

6.2.1.3 Alfred site

A field study was conducted from 2011 to 2014 in Alfred, Ontario (lat. 45.34° N, long. 74.55° W) to study the impacts of organic and inorganic fertilizer type and timing on silage corn growth, N loss to drains and N_2O emissions. The soil was a Bearbrook clay and tile drainage was present with hydrologically distinct plots. The average annual temperature at Alfred is 4.5 ^oC with 1021 mm average precipitation and 944 mm estimated PET making it by far the wettest of the three sites investigated. Other site properties are available in Table 6.1. The field study included six treatments and we chose the urea fertilized continuous corn silage treatment for our modelling approach assessments. Our current model version was recently setup for this site and the calibration and validation is documented in He *et al.* (2019b). Urea at the rate of 140 kg N ha^{-1} was surface applied then incorporated to 15 cm using a cultivator. Tile drains were installed at 90 cm depth and the plots were hydraulically isolated. Water flow and NO_3^- concentration to tile drains were monitored and daily values were recorded over a 2.5 year period. Composite soil samples were collected one to three times per month which were analysed for NO_3^- and NH_4^+. Silage dry matter yield and plant N content were measured at plant maturity. Nitrous oxide emissions were measured two to five times per month using non-steady-state chambers. Soil temperature and water contents were also measured frequently during the study. Further details of the site design, management and measurements are described by Schwager *et al.* (2016).

6.2.2 DNDC model description

The DNDC model was originally developed to simulate nitrous oxide emissions from agricultural systems (Li *et al.,* 1992) and gained attention due to its detailed biochemical processes used for estimating the impacts of microbial activity on nitrification and denitrification. It was later expanded to simulate soil C&N processes, N movement, ammonia volatilization and methanogenisis. The crop growth sub-model in DNDC has evolved over the last 20 years (Zhang and Niu, 2016) but it is still relatively simple. It primarily uses a GDD growth model with crop stress limitations due to water, nitrogen and temperature. The model simulates the impact of CO_2 fertilization on crop growth including the impacts of C assimilation in C3 and C4 crops, water and N use efficiency. DNDC uses the Penman Montieth approach for estimating evapotranspiration and includes a relatively simple cascade water flow approach for simulating water movement. DNDC can currently simulate a very large array of crops and management practices and several groups have worked on merging DNDC with other models or developing versions which demonstrate improved performance for regional conditions or specific processes (Gilhespy *et al.,* 2014).

In this study we employ a DNDC model version (DNDCv.CAN) which was originally developed to improve the simulation of crop cultivars and management in cool weather conditions (Kroebel *et al.,* 2011: Grant *et al.,* 2016), however, the model can still be applied in warmer agro-ecosystems (Ehrhardt *et al.,* 2018: Brilli *et al.,* 2017) since it includes an option to use default crop growth or crop parameters can be adjusted. Regarding impacts of climate change, Smith *et al.* (2013) lowered the effect of CO_2 fertilization on C assimilation, crop water and N use efficiency based on free-air CO_2 enrichment studies. Temperature stress on crop growth was revised based on an empirical equation derived in Canada (Yan and Hunt, 1999) and temperature stress during anthesis was included for maize, wheat, winter wheat (Smith *et al.,* 2013) and for legumes and perennials (He *et al.,* 2019a). Further developments focused on improving the simulation of evapotranspiration (ET; Dutta *et al.,* 2016b), ammonia volatilization (Congreves *et al.,* 2016), the effects of snow cover, crop residue and soil texture on soil temperature (Dutta *et al.,* 2018), and perennial growth and winterkill (He *et al.,* 2019a). The most recent developments involved a major restructuring of the model with a heterogeneous and deeper soil profile (0.5m to 2m), inclusion of root penetration and density functions, unsaturated flow and a new tile drainage sub-model (Smith *et al.*, 2019b). The model is available at https://github.com/BrianBGrant/DNDCv.CAN.

6.2.3 Model initialization, calibration and evaluation

Before attempting to simulate climate change impacts it is important to ensure that a model is well calibrated (Wallach *et al.*, 2019) and able to reasonable capture the impacts of inter-annual changes in weather on crop growth, soil carbon and reactive N losses. We chose research sites where a range of data was available for model calibration and validation. DNDC simulations were previously performed for the same cropping systems at each of the three research sites thus the necessary soil, climate and management inputs were readily available (Swift Current - Grant *et al.*, 2016, Woodslee - Jarecki *et al.*, 2018, Alfred – He *et al.*, 2019b) but in the case of Swift Current and Woodslee sites an older model version was employed thus we recalibrated our more recent version by using the similar approach of optimizing RMSE for outcomes using R language in a stepwise manner where parameters were adjusted. The details of each parameter are provided below. Climate data used for model calibration and validation during the experimental periods were available from on site weather stations. These variables included min and max temperature, precipitation, wind speed, solar radiation and relative humidity. The latest DNDC version including our hydrology developments was employed at Alfred thus we used the same inputs and parameterization as in He *et al.* (2019b) for all case study simulations.

At Woodslee a previous model version was used by Jarecki *et al.* (2018) thus we re-evaluated the latest version of DNDC for simulating long-term crop yields using the first 10 years of data for calibration (1959-1968) and the remainder for validation (1969-2105) in a similar manner as Jarecki *et al.* (2018). The RMSE of maize yields was minimized by adjusting the growing degree days from 2570 to 2800. The version of DNDC used in Jarecki *et al.* (2018) did not allow time for germination. Other maize parameters did not require modification and also the same parameterization as employed in Jarecki *et al.* (2018) was used for oats and (no observed yields available) and SOC. Alfalfa parameters were based on He *et al.* (2019a) since development for regrowth after cutting and in subsequent years was included in DNDC. Nitrous oxide emissions were calibrated slightly using data from rotational corn and the model was validated using data from monoculture corn (monoculture corn was included in 6 of 8 modelling approaches). The denitrifier bacteria growth rate was increased by 20% with no other adjustment. Parameterizations for the tile drainage sub-model were used from Smith *et al.* (2019b) who simulated water and N loss to runoff and tile drains at a nearby site with the same Brookston clay soil properties (Drury *et al.*, 2014b, long. 42°13'N, lat. 82°44'W).

At the Swift Current site the 50 cm version of DNDC was previously setup for simulating crop yields and SOC for the long term wheat and wheat-fallow rotations starting in 1967 (Grant *et al.*, 2016). In this study the same input data was used and the model was again calibrated for simulated crop yields using the wheat-fallow rotation and validated for monoculture. Note that N losses are very low for this semi-arid site, perhaps zero for N leaching below the root zone (Campbell *et al.*, 2006). To minimize RMSE for wheat yield the following changes to parameters were made. A rooting depth of 1.5 m was set for wheat as part of the new parameterization inputs and water demand was parameterized to be 325 g water/g DM. Thermal Degree Days was set to a value of 1600 and the C:N ratios for grain, leaf, stem and roots were set to 14, 80, 80 and 65 respectively.

6.2.4 Statistical measures for testing model performance and analysing differences between approaches

Model performance relative to observations for DNDC was evaluated using several statistical measures including root mean square error (RMSE), normalized RMSE (NRMSE) and the d index (Wilmott and Matsuura 2005**).**

$$NRMSE = 100\left(\frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(O_i-P_i)^2}}{\bar{O}}\right) \tag{6.1}$$

$$\mathrm{d} = 1 - \frac{\sum_{i=1}^{n}(P_i-O_i)^2}{\sum_{i=1}^{n}(|P_i-\bar{O}|+|O_i-\bar{O}|)^2} \tag{6.2}$$

where P_i is the predicted or simulated value and O_i is the observed value.

RMSE is commonly used to evaluate model performance for estimating yield and biomass. Jamieson *et al.* (1991) indicated that a model had excellent performance if NRSME < 10; good <

20; fair < 30; and poor > 30. The d index provides a qualitative assessment of model accuracy with $d \geq 0.9$ showing an "excellent" agreement between model and observed values, $0.8 \leq d \leq 0.9$ indicates a "good" agreement, $0.7 \leq d \leq 0.8$ a "fair" agreement and $d < 0.7$ a "poor" agreement.

Statistical analysis to determine whether there were any statistically significant differences between time periods and between management practices was conducted using one-way ANOVA analysis in the SPSS 25.0 package followed by the Duncan's test at the 0.05 level ($p < 0.05$).

6.2.5 Modelling approaches for simulating impacts of climate change on cropping systems

Several modelling approaches were simulated to compare common procedures used by the community and the relative impacts this methods may have on crop yields, N_2O emissions, N leaching and runoff, evaporation, transpiration and soil carbon change (Table 6.2). The impacts on NH_3 volatilization were not reported in this study since UAN fertilizer was injected at 10 cm depth and losses were near zero. The approaches are defined in Table 6.2 and are further described below.

Table 6.2 Modelling approaches simulated at the Swift Current, Woodslee and Alfred locations.

Approach	Approach description	Considerations
Base simulation	Detailed climate drivers; change planting and harvest schedule to optimize seasons; adjust fertilizer under climate change; no cultivar change; monoculture	Changes in cultivar and the impacts of rotation diversification were not included in our base simulation. There are almost unlimited options.
Minimum climate variables	Simple climate drivers (min/max temp and precipitation) versus fuller range of climate drivers (+solar radiation, wind speed, humidity)	A common approach in studies for assessing soil carbon and nitrogen cycling in cropping systems under climate change
Fixed fertilizer	Fixed fertilizer application rate over time based on current farming practices in a region	A common approach in many published climate change studies

Re-initialize soil	Re-initialization of soil C&N and water status after each simulation year	Re-initialization is often employed in model ensemble studies for assessing crop growth. Soil C&N feedbacks over time are not considered.
Fixed planting	Fixed planting and harvest schedule over time	A common approach in most large model inter-comparison studies.
Simple approach	Simple climate drivers, fixed planting and harvest and fixed fertilizer application rate	Represents a simple yet common approach for modelling climate change impacts on cropping systems
Alternative cultivar	Change crop cultivar to be better suited to changes in climate	Cultivars that currently require warmer regions with longer growing seasons for optimum growth were chosen
Crop rotation	Include the base crop in rotation with other crops	A rotation was chosen based on agronomy trials available at the research site.
Cultivar + crop rotation	Change crop cultivar to be better suited to changes in climate and include the base crop in rotation	An approach which includes adaptation to model climate change impacts on cropping systems

6.2.5.1 Base approach

The base simulation to which we then implement changes for each modelling approach includes detailed climate variables, adjusted planting dates to account for yearly changes in weather, and automated fertilize applictaion. This represents an approach which we have used in past studies (Jerecki *et al.*, 2018: Smith *et al.*, 2013) which includes important considerations for adjusting the simulation over time to account for changes in climate.

6.2.5.2 Adjustment of fertilizer rate

Under climate change modelling assessments or in any study whereby changes in management are investigated its important to adjust fertilizer application rates accordingly. For instance, if crop growth becomes subjected to more water and temperature stress over time then biomass will likely decrease and fertilizer rates should be adjusted downwards, similar to what a smart farmer would ensure. Otherwise additional N may be lost needlessly. We implemented a method in DNDC to adjust fertilizer rate over time to maintain similar crop N stress under changing management, soil conditions or climate. This is accomplished by calculating N rate based on spring inorganic soil N status and expected soil organic matter mineralization that will maintain a constant and small level of crop N stress derived over the previous 10-year running average. This method adjusts fertilizer N rate in a manner which would be reasonably consistent producer-based guidelines who use soil N testing.

6.2.5.3 Adjustment of planting date

Earlier planting dates for most crops are expected under climate change in Canada to avoid heat stress in critical growth stages such as during flowering and grain filling (Qian *et al.*, 2019). In this study planting date was adjusted using daily Tmax, Tmin and precipitation based on methodologies described in Bootsma and De Jong (1988) for spring wheat and on Bootsma and Brown (1995) for grain corn and corn silage. Harvest date was determined by the DNDC model whereby the crop was harvested shortly after maturity was reached.

6.2.5.4 Alternative cultivar selection

Potential changes in crop cultivars that may occur in the future are difficult to determine considering options for breeding and genetic modification. In our case we chose cultivars with qualities that exist in warmer regions of the US. Generally we chose cultivars with increased growing season length and optimum temperature in future periods, which would not perform well in todays climate. For instance, for spring wheat a typical cultivar grown in Canada currently has an optimum temperature of about 18 ℃ and requires 1600 growing degree days at base 0 degrees (GDD_0). We set the future cultivar characteristics in the 2070-2100 period to 2200 GDD_0 and optimum temperature of 22 ℃. These values were ramped up over time within each 30-year climate period. Spring wheat cultivars can range greatly in growing season length and optimum temperatures (Acevedo *et al.*, 2009). Our final cultivar in the 2070-2100 period has an average duration to maturity of 138.5 days which is consistent with the example provided in Acevedo *et al.* (2009) sown in May at 34°S, a considerable warmer location than Swift Current. Over the entire time period simulated (1981-2100) the characteristics of the corn cultivar at Woodslee were modified from 2750 to 3150 for GDD_0 and 5000 to 6000 for optimum grain C whereas silage corn at Alfred was modified from 2300 to 2600 for GDD_0 and 4950 to 5950 for optimum grain C production.

6.2.5.5 Impacts of crop rotation

To explore rotational impacts, including the feedbacks from residues of different crop types and changes in crop water use dynamics over time, the crop that was simulated under monoculture at each location (Swift Current: spring wheat, Woodslee: grain corn, and Alfred: silage corn) was included in a crop rotation relevant to the location. The rotations included 1) Swift Current: spring wheat-lentil, 2) Woodslee: corn-oats-alfalfa-alfalfa, and 3) Alfred: silage corn-silage corn-alfalfa-alfalfa. Note that the performance of DNDC for simulating crop yields and SOC for these rotations relative to measurements at Swift current and Woodslee is shown in Figs. 6.S1-6.S4. The rotation at Alfred was simulated by He *et al.* (2019b). Each phase of the rotations were simulated under climate change to enable reporting of yields, N losses and SOC for every year.

6.2.6 Climate data and climate change scenario

Climate data used for model calibration and validation during the experimental periods were available from on site weather stations. These variables included min and max temperature, precipitation, wind speed, solar radiation and relative humidity.

Downscaled climate projections from 1971 to 2100 were based on the CanRCM4 Global Circulation Model using the IPCC 8.5 watt m^{-2} radiative forcing representative concentration pathway (RCP) by the end of the 21st century (Fig. 6.S5). The historical weather data from each site was used for bias correcting the GCM simulations using a multivariate form of quantile mapping (Kirchmeier-Young et al., 2017; Cannon 2018). The RCP8.5 represents a future with relatively high GHG emissions (Van Vuuren *et al.*, 2011: IPCC 2014). In Canada, Jarecki *et al.* (2018) and He *et al.* (2018) found similar yet strong impacts of both the RCP8.5 and the more moderate RCP4.5 pathways on crop yields.

6.3 Results and Discussion

6.3.1 Evaluation of the DNDC model for simulating crop growth, SOC, N_2O, and N leaching

Before attempting to simulate the impacts of climate changes on cropping systems it is important to first ensure an agroecosystem model is responding reasonably in simulating the inter-annual impacts of climate drivers on crop growth, C&N cycling and N losses. In this study the three case study research sites were chosen because there was substantial data available for model calibration and evaluation and all three studies have previously been used to evaluate the DNDC model (Grant *et al.,* 2016: Jarecki *et al.,* 2018: He *et al.,* 2019b).

In this study the recent DNDC model version (Smith *et al.,* 2019b) performed reasonably in simulating crop yields, N leaching and N_2O at the 3 research sites. At the Swift current location spring wheat yields were well simulated with a d value of 0.95 indicating excellent performance (Table 6.3). Similar to previous evaluation (Grant *et al.,* 2016) the model responded well to inter-annual variations in precipitation for both monoculture and rotational wheat (Fig. 6.S1) and SOC was reasonably simulated (Fig. 6.S2) with an increase in SOC due to higher C inputs during a favorable climate period in the late 1990's when higher rainfall occurred. Very little if any N loss currently occurs below the root zone at Swift Current (Campbell *et al.,* 2006) in which DNDC was in agreement with no N leaching below 2m in the historical 1967-2009 period. Also, N_2O emissions at semi-arid locations such as Swift Current are typically small, usually being less than 1 kg N_2O-N ha^{-1} (Rochette *et al.,* 2018). Emission events are driven primarily by nitrification rather than denitrification since soil water content is low. In the historical period at Swift Current DNDC simulated average emissions of 0.45 kg N_2O-N ha^{-1}.

Table 6.3 Statistical evaluation of the DNDC model for simulating crop yields, N_2O emissions and N losses to tile drains at Swift Current, Woodslee, and Alfred Canada

Item	Site	Stage	Observed	DNDC	n	RMSE	NRMSE (%)	d
Crop yields (spring wheat and corn) or dry biomass (silage corn) (kg ha^{-1})	Swift Current	Calibration	2312	2581	43	678	29.3	0.95
		Validation	1630	1653	43	491	30.2	0.95
	Woodslee	Calibration	6106	5699	10	1220	20.0	0.81
		Validation	5947	6323	47	1343	22.6	0.78
	Alfred[1]	Calibration	13264	13111	4	194	4.70	0.98
		Validation	16510	15848	4	2274	13.7	0.98
Daily N_2O emissions (kg N ha^{-1})	Woodslee	Calibration	0.055	0.052	79	0.092	168	0.77
		Validation	0.049	0.042	79	0.085	174	0.81
	Alfred[1]	Calibration	0.005	0.005	114	0.010	192	0.88
		Validation	0.010	0.009	114	0.023	223	0.78
NO_3^- loss to tiles[2] (kg N ha^{-1})	Woodslee (n=28)	Calibration	3.14	3.18	28	2.70	85.9	0.82
		Validation	3.64	4.15	28	2.70	72.9	0.88
	Alfred[1] (daily)	Calibration	0.009	0.010	738	0.022	257	0.77
		Validation	0.047	0.040	738	0.084	180	0.78

[1] Model performance results for Alfred were adapted from He et al. (2019b)

[2] Model performance results for N loss to tiles at Woodslee were adapted from the unrestricted tile drainage treatments in Smith et al. (2019c)

The model performed "fair" to "good" in simulating corn yields under monoculture at Woodslee (Table 6.3; Fig. 6.S3a). The RMSE value of 1343 kg ha^{-1} was slightly lower than that achieved by Jarecki *et al.* (2018) using an earlier DNDCv.CAN model version and also the Decision Support System for Agrotechnology Transfer (DSSAT)-Crop Environment Resource Synthesis (CERES)-Maize model which produced an RMSE of 1391 kg ha^{-1} (Liu *et al.,* 2011). At this site rotational corn yields (corn-oats-alfalfa-alfalfa) were found to be higher than yields under monoculture (Jarecki *et al.,* 2018). Jarecki *et al.* (2018) found that the DNDC model could not originally simulate the differences in yields between the treatments but performed reasonably after a pedo-transfer function was incorporated to adjust water holding capacity based on changes in soil properties over time. This function is still active in the model employed in our study and the relative differences in yields between the treatments was again well simulated (Fig. 6.S3b). The difficulties in simulating the sometimes large year to year variability in yields may be due to high variability in weather and incidence of pests and disease which DNDC nor DSSAT includes. The DNDC model demonstrated "excellent" performance in simulating corn silage biomass at Alfred (He *et al.,* 2019b), albeit only 4 observations were available (Table 6.3).

DNDC showed similar performance at Woodslee and Alfred for simulating daily N_2O emissions with "fair" to "good" d values (Table 6.3). The performance was reasonable considering daily emissions can be sporadic due to heterogeneous variability in soil properties and differences in soil microbial populations. The current version of DNDC used in this study showed "good" performance in simulating N loss to tile drains at Woodslee (Smith *et al.,* 2019b) and "fair" performance at Alfred (He *et al.,* 2019b). The poorer performance at Alfred was attributed to difficulties in simulating complex snow accumulation and melt dynamics (He *et al.,* 2019b).

No observations of SOC were available at Alfred other than the initial values which were input into DNDC. At the Woodslee site observations were limited but DNDC performed well in predicting the differences in SOC levels between the monoculture corn (Fig. 6.S4a) and rotational corn-oat-alfalfa-alfalfa system (Fig. 6.S4b) in the 2004-2007 time period. For both cropping systems SOC at depth was within error bars of measurements except at the 20 cm depth where DNDC overestimated SOC concentration, which was an improvement over the simulations in Jarecki *et al.* (2018).

6.3.2 Overview of the simulated impacts of climate change on projected yields and N losses at the research sites

In Canada warming is occurring at about two times the rate of the global increase (Bush and Lemmen, 2019) thus it is not surprising that under the 8.5 Watt m^{-2} scenario we see large projected increases in temperature by the end of the twenty first century (Table 6.4, Fig. 6.S5). This higher temperature can adversely impact crop yields through temperature stress, especially during critical growth phases, however, this can be offset by changing planting time (Qian *et al.*, 2019). Also, a projected increase in rainfall (Table 6.4, Fig. 6.S5) and higher crop water use efficiency under elevated CO_2 can offset increased potential evapotranspiration. In many cases crop yields are projected to increase under future in Canada (Qian *et al.*, 2019: He *et al.*, 2018a: Smith *et al.*, 2013) and our current model assessments are consistent with this finding at the Swift Current and Alfred locations. At each of the three study locations increased seasonal GDD is projected to occur in the future with crops reaching maturity more quickly. For our base modelling approach planting time was adjusted to an earlier date to reduce temperature stress during critical phases and fertilizer rates were automatically increased at Swift Current and Alfred to account for higher crop growth under the projected favourable future climate.

Table 6.4 Projected weather for 8.5 W m^{-2} IPCC scenario, estimated changes in management and impact on crop yields for the base simulation at Alfred, Woodslee and Swift Current, Canada

Location	Period	Precip. (mm)	Avg. annual temp. (mm)	PET# (mm)	Trans# (mm)	Evap# (mm)	Total available seasonal GDD*	Average planting date (M/D)	Average harvest date (M/D)	Time to reach maturity (days)	Fertilizer application rate (kg N ha^{-1})	Crop yield or dry biomass (Mg ha^{-1})^
Swift Current	1981-2010	349	4	1131	105	228	2430	01-May	01-Sep	123	45	1.63
(spring wheat)	2011-2040	361	6.3	1243	117	225	3018	13-Apr	12-Aug	121	55	1.78
	2041-2070	398	7.9	1301	141	234	3387	10-Apr	04-Aug	115	74	2.51
	2071-2100	423	10.5	1431	171	222	3992	06-Apr	25-Jul	110	105	3.1
Woodslee	1981-2010	845	9.3	1046	181	268	3146	02-May	07-Oct	158	119	6.02
(corn)	2011-2040	854	11.3	1144	170	298	3676	15-Apr	12-Sep	150	114	6.13
	2041-2070	980	12.7	1192	155	318	4027	12-Apr	31-Aug	142	119	6.14
	2071-2100	941	15	1277	134	332	4592	10-Apr	18-Aug	130	112	5.78
Alfred	1981-2010	923	6.7	944	291	234	2713	07-May	21-Sep	136	106	14.6
(corn silage)	2011-2040	917	8.4	1012	277	253	3103	01-May	06-Sep	128	118	14.8
	2041-2070	1011	10.2	1080	286	262	3574	27-Apr	24-Aug	119	138	16.8
	2071-2100	1096	12.7	1162	269	291	4153	21-Apr	11-Aug	111	148	17.5

*Potential GDD during the growing season calculated at base 5°C for spring wheat and 10°C for grain corn and silage corn.
#Potential Evapotranspiration, simulated actual Transpiration and simulation actual Evaporation
^ Corn silage is shown in units of dry matter.

In Figs. 6.1-6.3 boxplots are provided to show the impacts of selected modelling approaches during four 30-year time periods at the three research sites. Each boxplot shows the model result across 30 years of climate variability simulated continuously. It is apparent that many of the modelling approaches strongly impacted projected yields and N losses. Average yields for the base approach at Swift Current were projected to increase over time and they were strongly influenced by inter-annual variability in precipitation which is consistent with simulation results from several studies (Qian *et al.*, 2019: He *et al.*, 2018b: Smith *et al.*, 2013) (Fig. 6.1). Yields at the upper 95th confidence interval in the 1981-2010 historical period were almost double of the average yields. The largest variability occurred in the 2071-2100 time period, which was also true for projected N losses at Swift Current. Note that all modelling approaches, except for fixed fertilizer and the simple approach, showed at increase in spring wheat yields under climate change, but yields differed in magnitude. The decline in yield variability when fertilizer rate was fixed (also included in simple approach) was caused by crop N stress due to limited N availability (see section 3.3.2 for more detail). Though N losses at this semi-arid location were low, greater and more variable N_2O emissions, N leaching and N runoff were generally predicted to occur in future periods. This was mainly caused by increased microbial activity under a warmer climate impacting the mineralization, nitrification, and denitrification processes in DNDC.

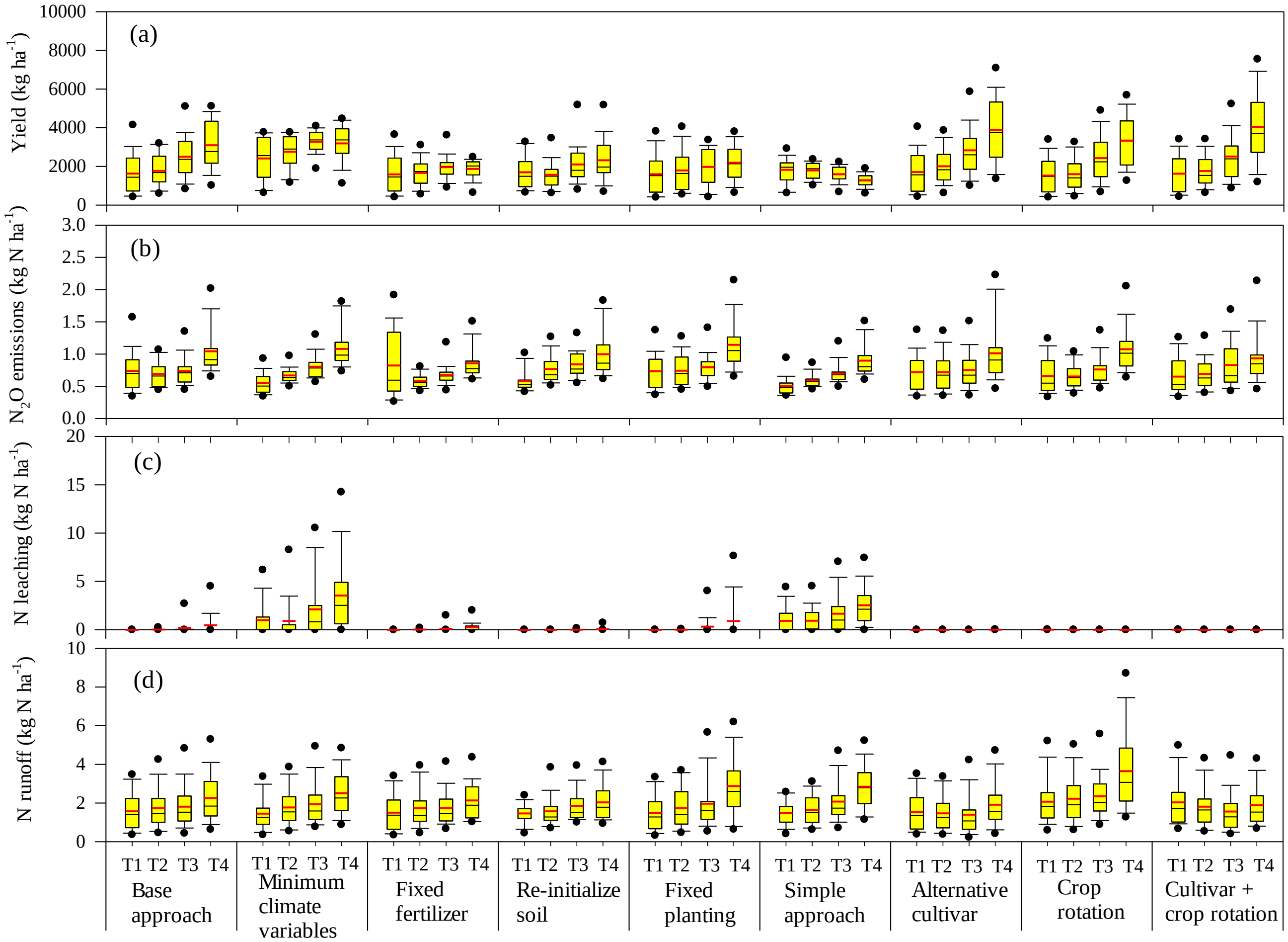

Figure 6.1 Boxplots showing impacts of selected modelling approaches across 30 years of climate variability at the Swift Current location on a) spring wheat yield, b) N_2O emissions, c) N runoff, and d) N leaching to tile drains. The black and red lines, lower and upper edges of the boxes, bars and dots represent median and mean values, 25th and 75th, 5th and 95th, and <5th and >95th percentiles of all data, respectively. T1, T2, T3 and T4 represent the time periods 1981-2010, 2011-2040, 2041-2070, and 2071-2100, respectively.

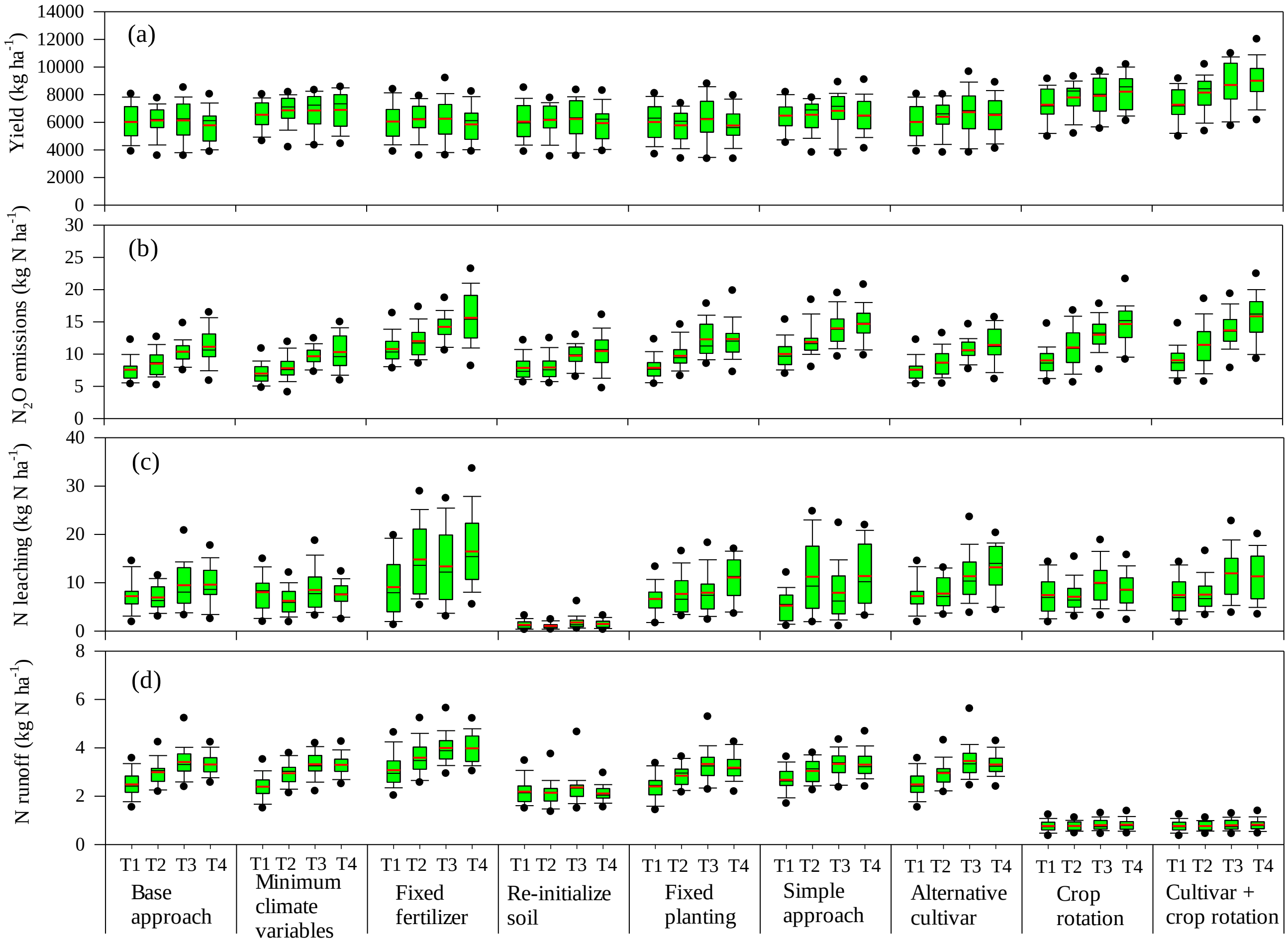

Figure 6.2 Boxplots showing impacts of selected modelling approaches across 30 years of climate variability at the Woodslee location on a) grain corn yield, b) N_2O emissions, c) N runoff, and d) N leaching to tile drains. The black and red lines, lower and upper edges of the boxes, bars and dots represent median and mean values, 25th and 75th, 5th and 95th, and <5th and >95th percentiles of all data, respectively. T1, T2, T3 and T4 represent the time periods 1981-2010, 2011-2040, 2041-2070, and 2071-2100, respectively.

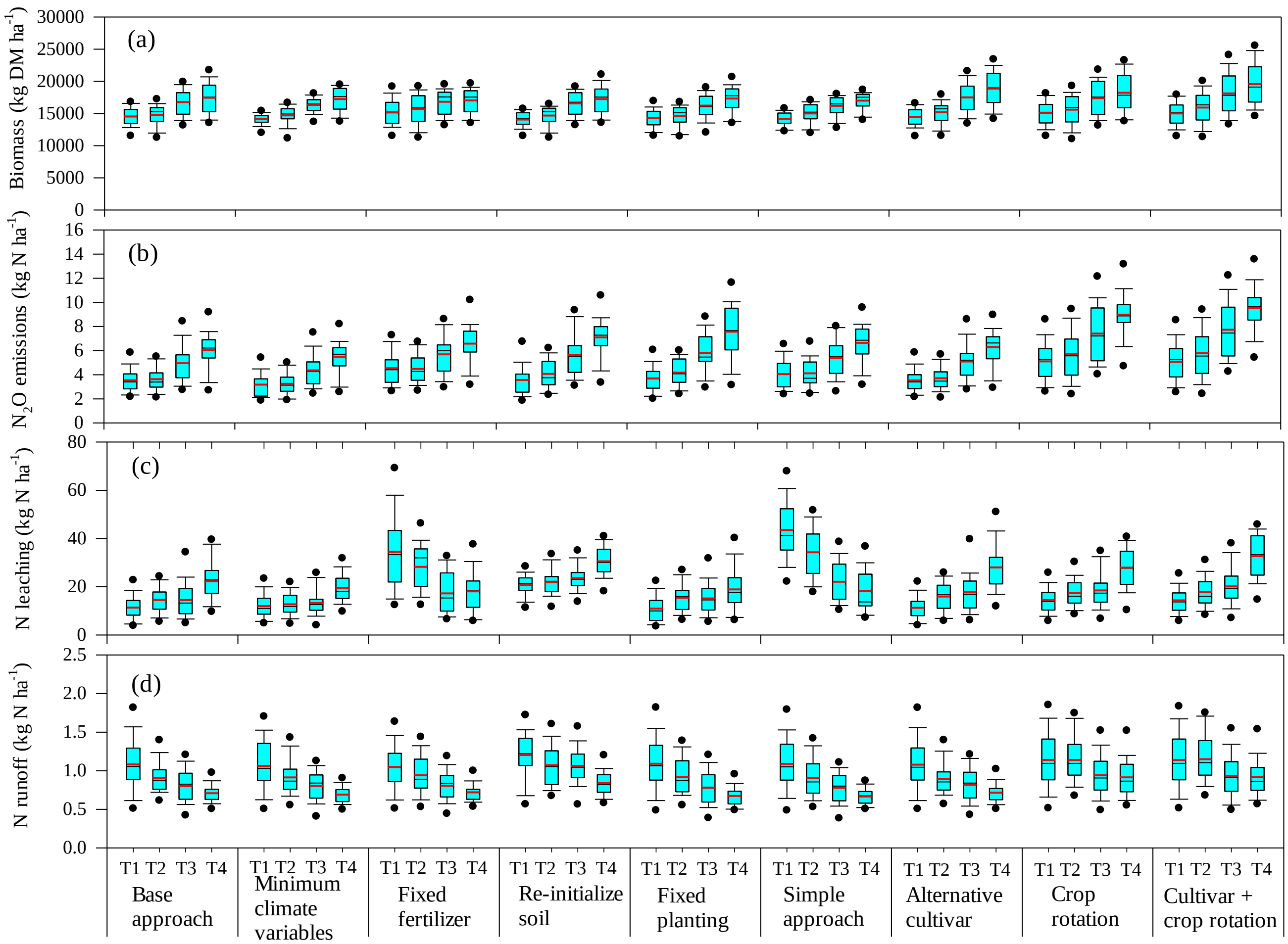

Figure 6.3 Boxplots showing impacts of selected modelling approaches across 30 years of climate variability at the Alfred location on a) corn silage above ground dry biomass, b) N_2O emissions, c) N runoff, and d) N leaching to tile drains. The black and red lines, lower and upper edges of the boxes, bars and dots represent median and mean values, 25th and 75th, 5th and 95th, and <5th and >95th percentiles of all data, respectively. T1, T2, T3 and T4 represent the time periods 1981-2010, 2011-2040, 2041-2070, and 2071-2100, respectively.

For the base approach at Woodslee, as well as other approaches which employed monoculture cropping, no significant changes in corn yields were projected under climate change but increases in yields were projected for rotational corn (Fig. 6.2). The variability in yields remained relatively constant from 1981-2100. At this location average temperature is highest resulting in more heat stress during growth in the future. Also, more water stress occurred than at the Alfred site, due to less precipitation and higher PET. Using DNDC, Jarecki *et al.* (2018) similarly predicted that corn in monoculture did not increase in yields under future climate but when corn was grown in rotation water stress was mitigated resulting in trends in higher yields.

Similar to Swift Current the predicted magnitude and variability in N losses at Woodslee tended to increase under future climate change with N_2O increasing by about 50% by the 2071-2100 period for the base approach. The projected increase in N_2O emissions under climate change is consistent with other model assessments in Canada (Smith et al., 2013), the United States (Tian *et al.*, 2012) and South West England (Abalos *et al.*, 2016a).

At Alfred higher corn silage biomass was predicted in the future (Fig. 6.3). The location has cooler climate and 155 mm more average precipitation in the 2071-2100 period than at Woodslee (Table 6.4). The relative increase in silage biomass was not as dramatic as the increases for spring wheat yields at Swift Current but corn is a C4 crop for which CO_2 fertilization only has a minor impact on C assimilation, which is included in DNDC (Smith *et al.*, 2013) based on free-air CO_2 enrichment studies (Long *et al.*, 2006: Leakey *et al.*, 2009). At Alfred N_2O emissions also increased under climate change for all approaches, but the magnitude differed between approaches. Nitrogen leaching increased for the base approach but when fixed fertilizer was employed leaching was high in the 1981-2010 period followed by a decline in future periods. Interestingly, unlike the other locations N runoff was predicted to decline in future periods and this was caused by reduced snow cover in the future thus reduced N runoff during snowmelt (Fig. 6.S6). Average N runoff in the spring (Jan 1 to April 30) declined from 0.53 kg N ha^{-1} in the 1981-2010 time period to 0.20 kg N ha^{-1} in the 2071-2100 period, yet growing season runoff (May 1 to Oct 31) did not change (0.39 to 0.41 kg N ha^{-1} in the respective time periods). Currently, much greater snow cover occurs at Alfred than at the other locations due to higher winter precipitation and cooler winter temperatures than at Woodslee.

6.3.3 Comparison of approaches for modelling the impact of climate change on cropping systems

6.3.3.1 Minimum climate variables

Average differences between each approach and the base approach for each respective time period, 1981-2010, 2011-2040, 2041-2070 and 2071-2100, are shown in Figs. 6.4-6.6 for each location. At Swift Current the approach whereby we used only minimum and maximum temperature and precipitation as climate variables resulted in significantly higher yields (Table 6.S1) than the "base approach" from 1981-2070. This was because the predicted evaporation (Fig. 6.S7) was much lower resulting in less crop water stress. The DNDC model uses an FAO approach to estimate radiation when it is not available which usually results in good seasonal estimates of ET but poor daily correlation. However, DNDC uses a constant wind speed of 2 m s^{-1}, which is reasonable for some eastern locations, but evaporation is underestimated at Swift Current since the average wind speed is 7.4 m s^{-1}. It is likely that other crop models also use simplified approaches when a fuller range of weather inputs are not available. The DNDC model previously used a Thornthwaite approach to estimate ET which did not use wind speed, but ET was poorly estimated and the algorithm was replaced with a Penman Montieth approach using crop specific coefficients (Dutta *et al.*, 2016b). In the 2071-2100 time period evaporation was still predicted to be low but yields were only slightly higher than the base approach, being limited by biomass potential. A similar impact of using only temperature and precipitation as inputs was apparent for corn production at the Woodslee location where yields were projected to be 14 % higher on average from 2011 to 2100 than the base approach (Fig. 6.5, Table 6.S2) and evaporation was lower (Fig. 6.S7). At Alfred (Fig. 6.6, Table 6.S3) evaporation was also lower but there was very little change in yields, generally because the crop experienced less water stress at this location. The simple climate approach resulted in significantly greater N leaching at Swift Current where leaching was increased from near zero for the base approach to 3.5 kg ha^{-1} in the 2071-2100 period (Fig. 6.4, Table 6.S1). This may have been caused by higher residue inputs to the soil resulting in higher SOC (Fig. 6.7) and greater mineralization. Nitrogen losses were not significantly impacted at Woodslee and Alfred (Table 6.S2, 6.S3) though the model did appear to simulate a small and consistent reduction in N_2O emissions between time periods which was caused by higher soil water contents (less evaporation) pushing the denitrification reaction to N_2, rather than N_2O.

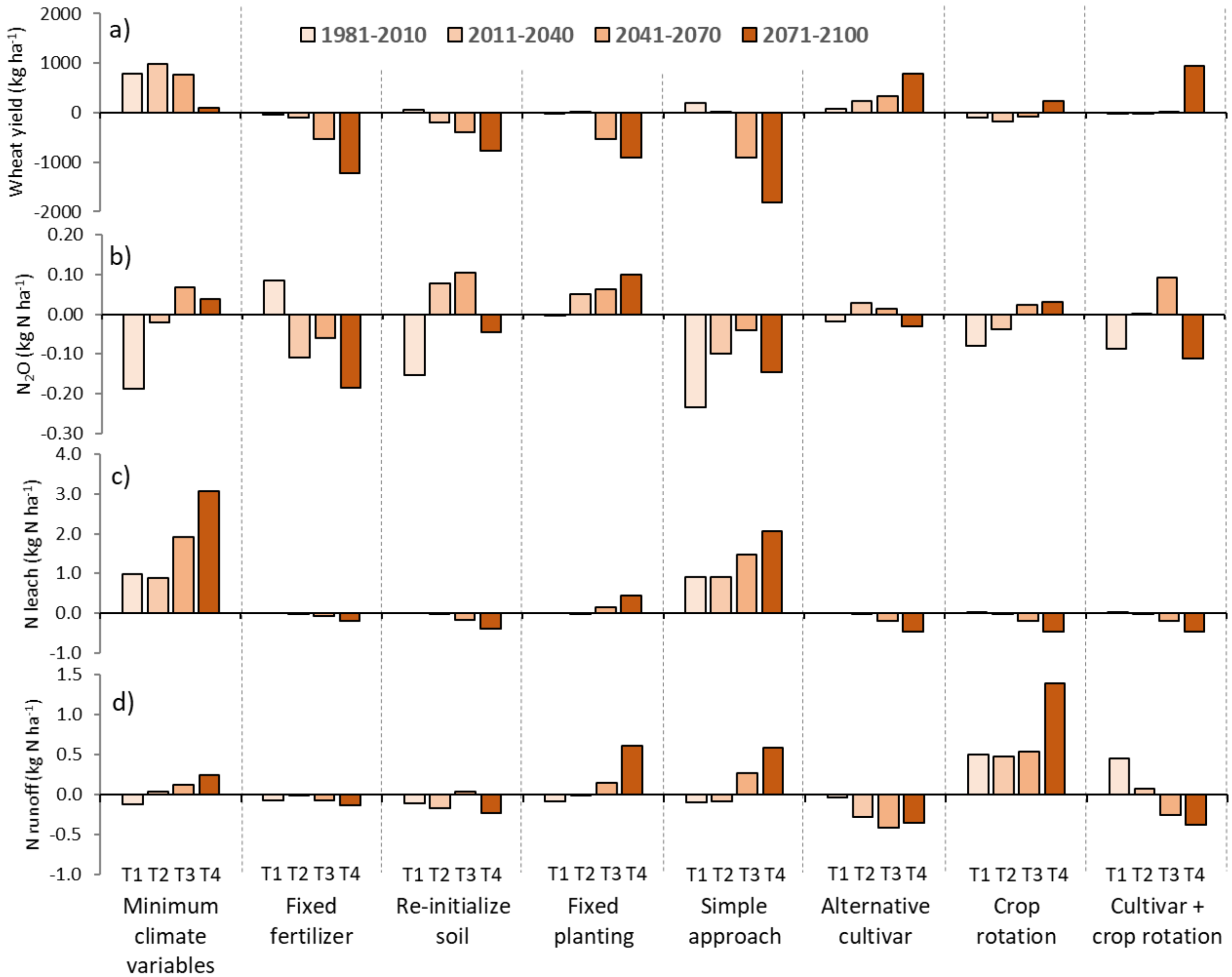

Figure 6.4 Difference in a) yield, b) N_2O emissions, c) N loss to tile drains, and d) N runoff between the exploratory modelling approaches and the base approach at the Swift Current location. T1, T2, T3 and T4 represent the time periods 1981-2010, 2011-2040, 2041-2070, and 2071-2100, respectively.

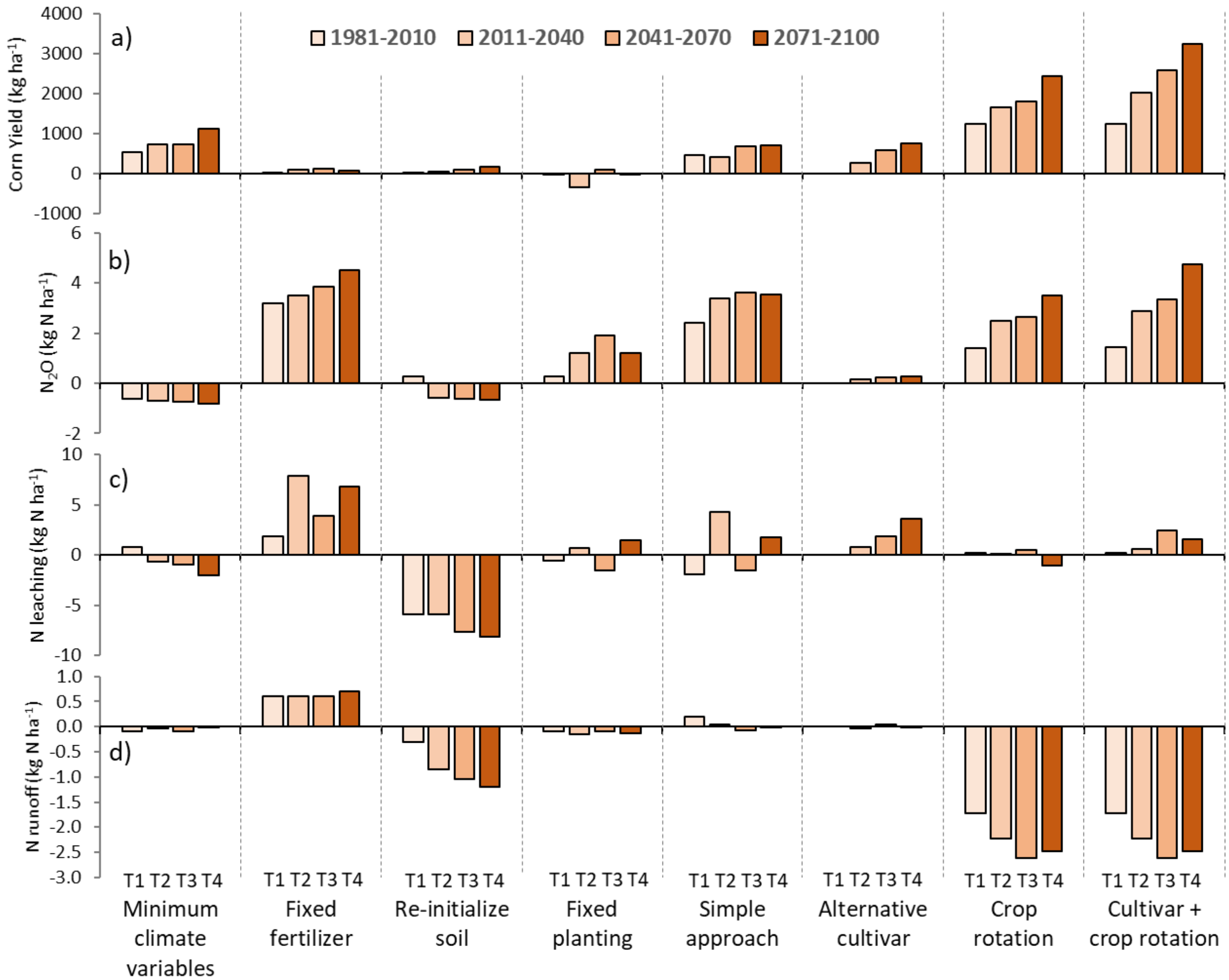

Figure 6.5 Difference in a) yield, b) N_2O emissions, c) N loss to tile drains, and d) N runoff between the exploratory modelling approaches and the base approach at the Woodslee location. T1, T2, T3 and T4 represent the time periods 1981-2010, 2011-2040, 2041-2070, and 2071-2100, respectively.

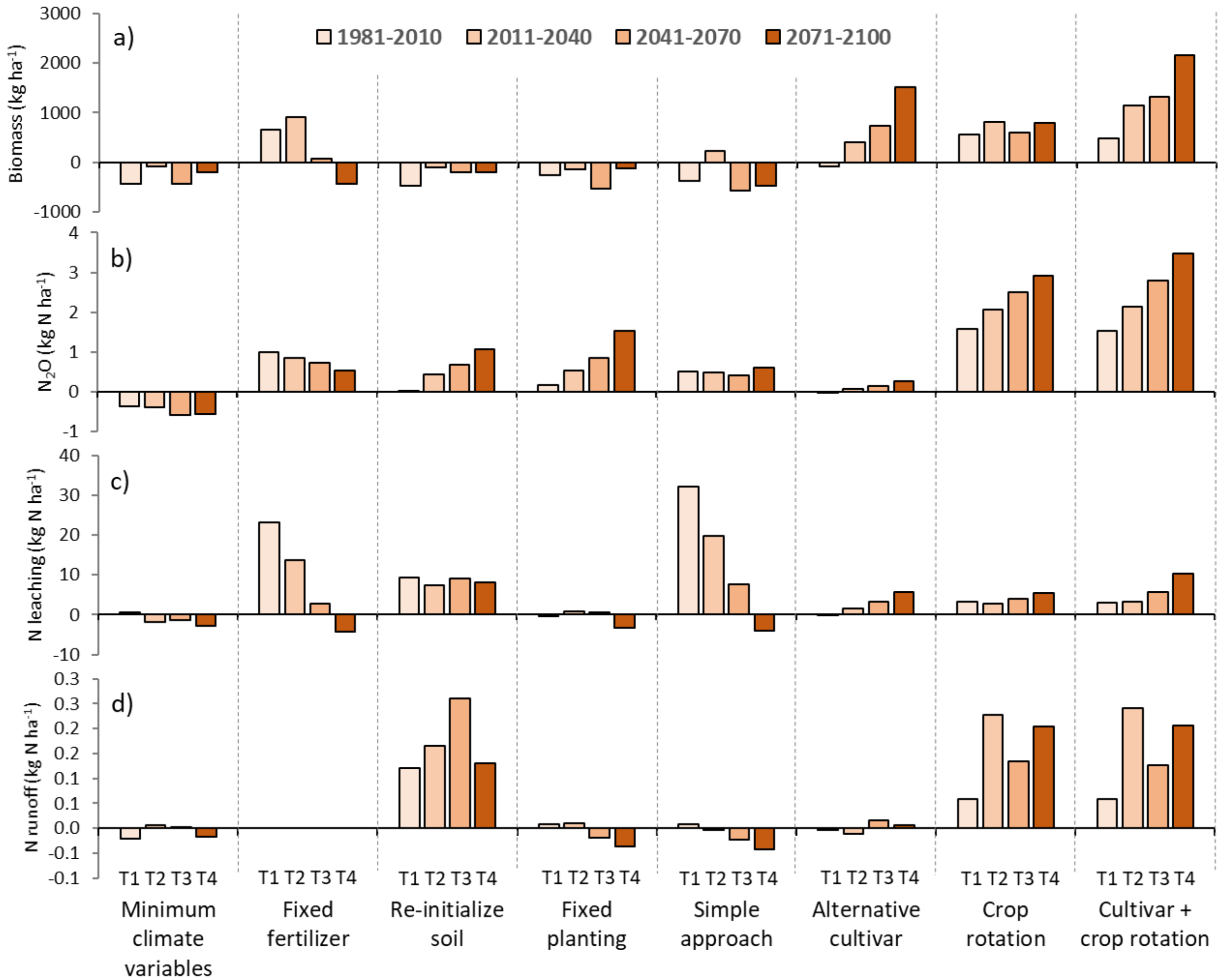

Figure 6.6 Difference in a) yield, b) N_2O emissions, c) N loss to tile drains, and d) N runoff between the exploratory modelling approaches and the base approach at the Alfred location. T1, T2, T3 and T4 represent the time periods 1981-2010, 2011-2040, 2041-2070, and 2071-2100, respectively.

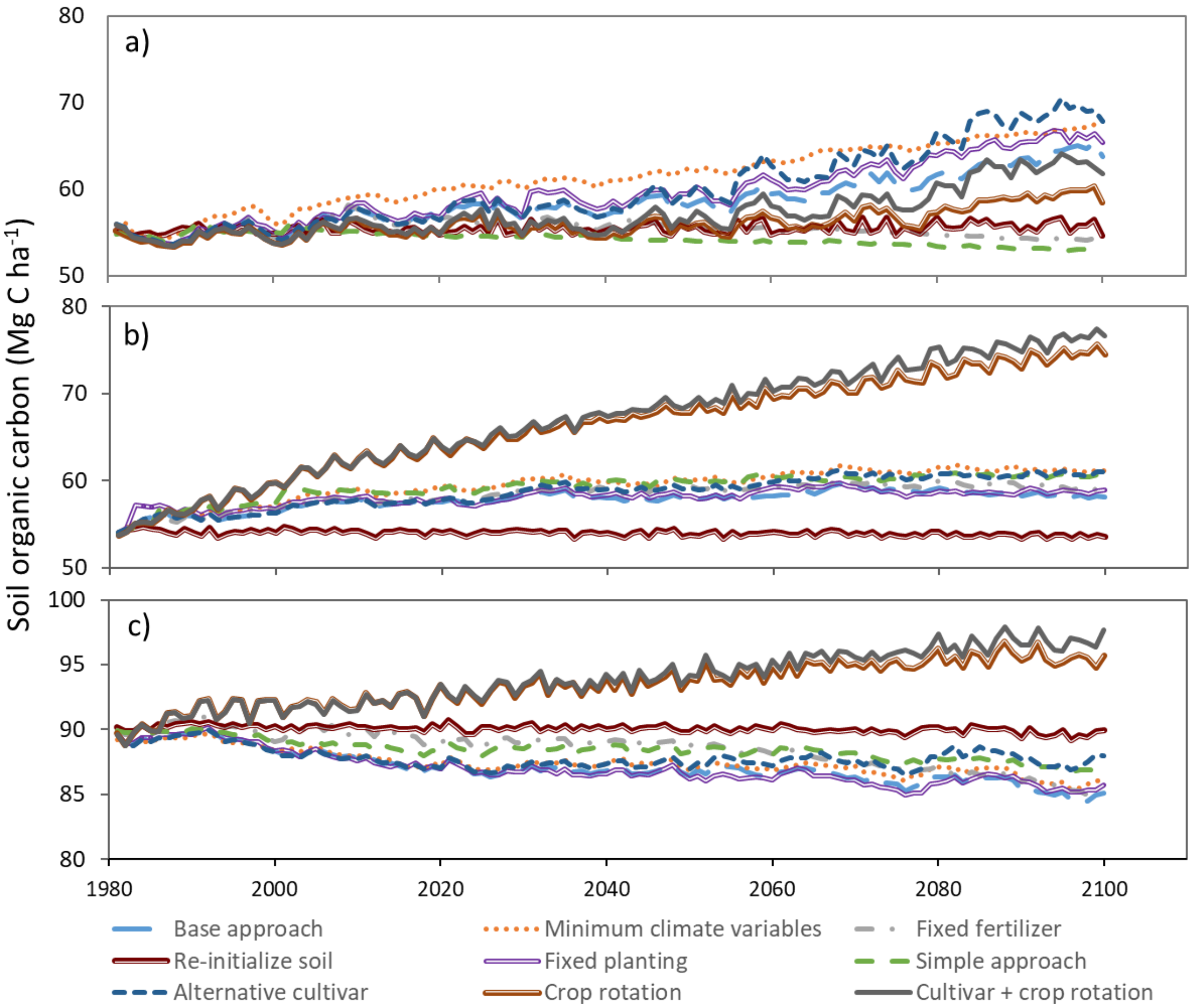

Figure 6.7 Simulated total soil organic carbon to 2 m depth for each modelling approach at the a) Swift Current, b) Woodslee and c) Alfred locations from 1981 to 2100.

6.3.3.2 Fixed fertilizer

Simulation of fixed fertilizers rates over time is common in many published climate change modelling studies (He *et al.,* 2018a: Abalos *et al.,* 2016b) but there is concern regarding the results. If adverse conditions for crop growth occur in the future then there will be excess soil N and higher N losses than plausible. It is likely that farmers would adjusted fertilizer rate to a reasonable amount. On the other hand, if the climate becomes more favorable then growth will be limited and grain quality may decrease due to N stress. In this case future N losses may be underestimated. For sensitivity analysis, such as assessment of crop interactions for ranges of atmospheric CO_2 concentration, Temperature, and Water (CTW) performed in the Agricultural Model Intercomparison and Improvement Project (AgMIP; Mcdermid *et al.,* 2015), the use of fixed fertilizer rates can impose an issue. The response of a model to improved weather including the impacts of CO_2 fertilization can be greatly restrained when fertilizer is limited.

At Swift Current climate is projected to become more favorable for wheat production in the future but to accomplish this increased growth considerably more fertilizer is needed. An example showing the high simulated variability in spring wheat yields, increased yields over time and the automated adjustment of fertilizer application rates from 1981 to 2100 is shown in Fig. 6.8. High inter-annual variability in yields is typical in the semi-arid prairies where crop water stress is prevalent in some years (Grant *et al.,* 2016). In the period from 1981 to 2020 the fixed rate of 45 kg N ha^{-1} generally provided sufficient N for the crop growth, however, as climate became more favorable over time more N was required to meet the higher crop N demands thus yields were greatly reduced under the fixed application scenario. There was little change in N losses since N losses were already very low at Swift Current under the base scenario (Fig. 6.4). However, SOC was greatly reduced in comparison to the base approach due to less C inputs from crop residues (Fig. 6.7). It becomes apparent that its crucial for climate change assessment studies to adjust fertilizer rates over time, especially when there is either a large positive or negative feedback of climate drivers.

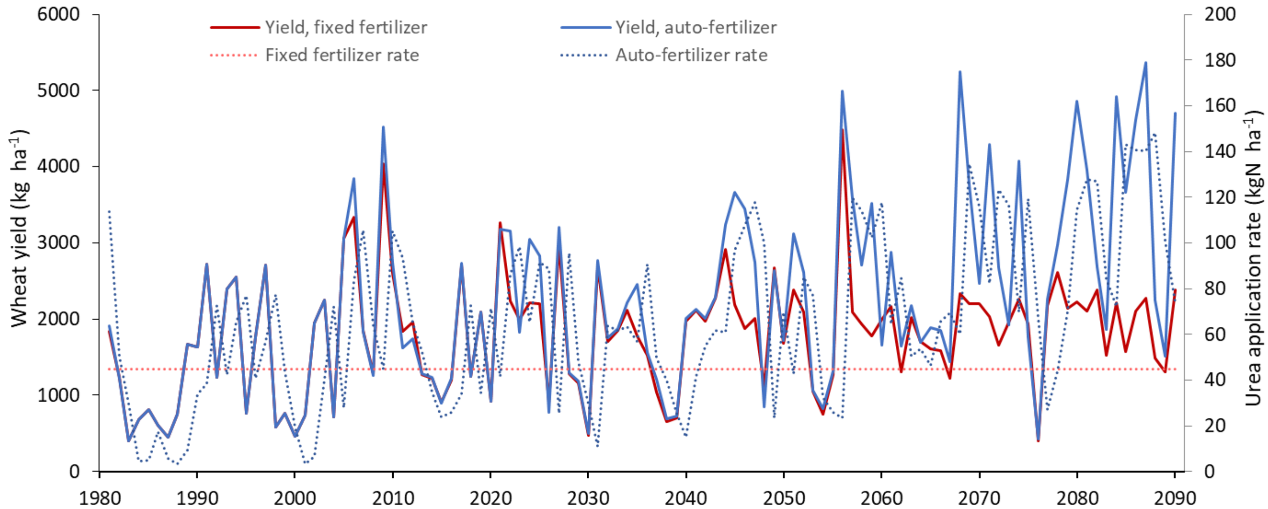

Figure 6.8 Simulation of fixed versus automatic fertilization (base approach) for spring wheat under the 8.5 W m^{-2} IPCC climate change scenario at Swift Current, Saskatchewan

Interestingly, corn yields/biomass did not change much at the Woodslee or Alfred locations (Figs. 6.5, 6.6). At Woodslee the climate was not more favorable for monoculture corn production in the future periods thus similar fertilizer rates were required. At Alfred more crop N demand was apparent over time, however, the soil initially had a very large store of organic C&N due to a long history of manure slurry application.

Fixed fertilizer resulted in much higher N_2O emissions and Woodslee and Alfred (Figs. 6.5, 6.6), particularly at Woodslee where emissions were projected to significantly increase by approximately 40% across all future periods (Table 6.S2). This was because the application rate was not adjusting according to soil N status each year, thus in certain years there was excess N and high emissions. Likewise there was significantly greater N leaching and N runoff in most time periods at Woodslee. A contributing factor is that DNDC includes the impacts of elevated CO_2 on the reduction in leaf N due to Rubisco acclimation (Leakey *et al.*, 2009), thus less N is required to produce the same quantity of biomass. The fixed fertilizer approach at Alfred resulted in significantly increased N_2O emissions and N leaching from 1981-2040 (Table 6.S3), but in later time periods not enough N was applied to meet the increased biomass potential thus N losses were no longer increased over the base approach.

6.3.3.3 Re-initialization of soil status each year

Re-initialization of soil status each year is a common practice employed in crop modelling (Basso *et al.*, 2015) but it is less common in studies which simulate reactive N losses and is not feasible for assessing long-term SOC dynamics. The method is likely used to overcome model limitations whereby long-term soil C&N dynamics and over-wintering processes are not effectively simulated. Our current study demonstrates that uncertainty is introduced when using this method. Re-initialization of the soil status each year results in no inter-annual feedbacks of crop residue inputs on SOC (Fig. 6.7) or soil N and water status. Thus when using this approach there is reduced impacts of climate change on crop production in subsequent years. At Swift Current re-initializing soils each year had a very strong impact on crop yields. Model simulations indicated that crop growth was adversely impacted over time with a significant 25% reduction in yields by the 2071-2100 period (Fig. 6.4, Table 6.S1). Note that in DNDC changes in soil water holding capacity are estimated over time based primarily on soil organic matter content (Jarecki *et al.*, 2018) which is driven by C inputs. Thus when the soil is reset reducing the feedbacks from potentially increased residue C inputs the model predicts more crop water stress and less growth. At the Woodslee and Alfred locations crop yields and biomass are only weakly impact by resetting soil status each year (Figs. 6.5, 6.6). This is partly because crop growth is not as severely water stressed at these sites, but also, auto-fertilization compensates for the lack of feedbacks from soil C&N cycling. At Woodslee SOC increases under the base approach providing more inputs from mineralized N than when the soil is reset each year whereas at Alfred the opposite is the case (Fig. 6.7). Thus when the soil is reset the auto-fertilization algorithm in DNDC compensates by applying on average 22% more fertilizer at Woodslee (because the N from mineralization is lacking relative to the base approach) and 16% less at Alfred. A fixed fertilizer rate coupled with resetting the soil status results in a decline in yields at Woodslee (data not shown).

Decreased decomposition of residues when the soil is reset each year at the Woodslee site results in significantly less annual N leaching and N runoff in all time periods (Fig. 6.5, Table 6.S2). Although the auto-fertilization routine alleviates crop N stress there is still less N in the soil profile for most of the year relative to the base approach, particularly in the non-growing season period when N is known to be subject to leaching and runoff in cool weather conditions (Smith *et al.*, 2019a: Gamble *et al.*, 2018: Schwager *et al.*, 2016). At Alfred we see the expected opposite impact with more N leaching and runoff under the soil re-initialization approach (Fig. 6.6). This is because SOC levels are higher and more N mineralization occurred than under the base approach. The differences were again significant across all time periods and also N_2O emissions were significantly higher in the 2170-2100 period (Table 6.S3).

6.3.3.4 Fixed planting

Obviously, the adjustment of planting time to an earlier period when heat stress is less likely to be incurred can reduce adverse impacts of climate change and improve crop growth. At Swift Current there was a 20.9 and 29.2 % projected average reduction in crop yields when planting date remained fixed relative to adjusting planting dates in the 2041-2070 and 2071-2100 periods, respectively (Fig. 6.4, Table 6.S1). The reduced yields with less crop N uptake resulted in slightly increased N_2O emissions, N leaching and N runoff. These losses would have been much higher if auto-fertilisation (reduced fertilizer rates) was not employed to compensate for the lower crop N requirements in the fixed planting date scenario. Due to lower C inputs, SOC was lower than the base approach (Fig. 6.7).

At Woodslee there was little discernable differences in yields when planting time was adjusted (Fig. 6.5). There was a small simulated reduction at Alfred for each time period (Fig. 6.6) but the change was not significant (Table 6.S3). Less crop water stress occurs at the humid locations than at Swift Current and corn has a much higher optimum temperature than spring wheat thus the adjustment in planting date does not strongly impact corn growth. It is, however, expected that planting date adjustment would strongly influence growth of small grains at these humid locations, since they have lower optimum temperatures and would be subject to increased heat stress during anthesis. No significant change in N runoff or leaching occurred at Woodslee or Alfred, however, N_2O emissions were sometimes significantly higher under the fixed planting approach at both sites in the 2041-2070 period and also at Alfred in the 2071-2100 period (Tables 6.S2, 6.S3). This was because fertilizer was applied at the time of planting and soil temperature was warmer under the fixed planting scenario. Temperature is a strong driver of nitrification and denitrification activity.

6.3.3.5 Simple approach

At Swift Current the simple approach resulted in very low simulated yields in the future periods, -58% relative to the base approach in the 2071-2100 period (Fig. 6.4, Table 6.S1). This was compounded due to employing both fixed planting and fixed fertilizer rates in the simulations, approaches which both lowered yields, offsetting the increased yields from using simple climate variables that produced lower ET (Fig. 6.S7). We also found significantly greater N leaching in all four time periods (Table 6.S1) which was primarily due to the use of simple climate where we had less evaporation and more water movement to the deeper profile.

At Woodslee and Alfred there was a similar response in yields and biomass as the simple climate approach (Figs. 6.5 and 6.6), with higher yields at Woodslee than the base approach due to less ET and crop water stress (Fig. 6.S7). At Woodless nitrous oxide emissions were significantly higher in all time periods than the base approach, being on average 35% higher (Table 6.S2). At Alfred N leaching was significantly higher from 1981-2070 (Table 6.S3) due primarily to the application of fixed fertilizer rates. Auto-fertilization applies N based on crop needs annually.

6.3.3.6 Impact of including an alternative cultivar

In Canada it is expected that longer growing season length will be realized under climate change (Qian *et al.*, 2013) and 2-3 weeks greater length has already been realized (Qian *et al.*, 2012). The simulation results indicate that in the future it may be possible to grow crop cultivars which require greater heat units. As expected, yields increase from 2011 to 2100 at all three locations (Figs. 6.4-6.6) with significantly increased spring wheat yields (26%) at Swift Current (Table 6.S1). Even though soil carbon increased greatly, especially in the 2071-2100 period (Fig. 6.7), nitrogen losses at Swift Current remained small and relatively similar to the base approach. At Woodslee and Alfred significantly greater N leaching occurred in the latter time periods being caused by higher fertilizer application rates to meet the crop N demands of the alternative cultivar (Tables 6.S2, 6.S3). In our case we only employed cultivars that currently exist. The extent to which crop water requirements, resistance to heat stress and resistance to disease could be modified through breeding and genetic modification in the future is unknown.

6.3.3.7 Impact of crop rotation

The growth of a crop can be impacted by rotational effects such as changes in soil properties soil nutrient and water status due to differences in crop root structure and C&N feedbacks over time (St Luce *et al.,* 2019: Jarecki *et al.,* 2019). The DNDC model simulates changes in soil water holding capacity over time based on changes in soil properties (Jarecki *et al.,* 2018). At Woodslee and Alfred we simulated an expected increase in SOC when alfalfa was included in rotation (Fig. 6.7) and this had an impact on reducing water stress on corn production. This was apparent in the historical model validation period at Woodslee (Fig. 6.S3) and at other locations in Canada (Lychuk *et al.,* 2019: Jarecki *et al.,* 2018). Corn yields at Woodslee were highly impacted when a diverse rotation was considered with yields increasing by up to 31.6% in the 2071-2100 time period (Fig. 6.5) with significant increases in all four time periods (Table 6.S2). At Alfred where less water stress was apparent the rotational impacts were smaller with silage biomass increasing by only a few percent (Fig. 6.6). At Swift Current there was a small decline in SOC (Fig. 6.7) as time progressed with no significant change in wheat yields (Table 6.S1) for the wheat-lentil rotation relative to the base approach (with monoculture spring wheat). In this case DNDC simulated similar C inputs from lentil as spring wheat, but a slightly accelerated loss of SOC due to higher N content of the lentil residues. This is also a finding of St Luce *et al.* (2018) when lentil green manure was incorporated in a study performed at Swift Current. DNDC also does not include the impact of high temperature stress on grain production for the lentil crop whereas it does for the other crops simulated in this study, thus the model may be underestimating the amount of residue returned to the soil as harvest index is not reduced for lentil under the higher temperatures.

At Swift current little change in N_2O emissions or N leaching occurred under rotational wheat-lentil. A small amount more N runoff occurred, being significant in the 2071-2100 period (Table 6.S1). At Woodslee and Alfred there was significantly greater N_2O emissions in all time periods for rotational corn and rotational corn silage than under monoculture (Figs. 6.5, 6.6). Higher emissions are known to sometimes occur in the year following plow down of alfalfa (Uzoma *et al.,* 2015) but note that the average simulated annual emissions during the entire rotation (including alfalfa) was lower than under monoculture. At the Woodslee location observed N_2O emissions from rotational corn were 12% higher on average than under monoculture (Table 6.3; rotational corn was used for model calibration). Nitrogen runoff was found to be significantly lower under rotational corn than monoculture at Woodslee which was consistent with site observations (Woodley *et al.,* 2018). This was mainly because the model simulated higher soil water holding capacity at higher SOC contents (Fig. 6.7) for rotational corn and greater infiltration occurred due to higher surface hydraulic conductivity based on values taken from Woodley *et al.* (2018). At Alfred N runoff increased by a small amount relative to monoculture but SOC and the related soil water holding capacity did not increase as drastically as at Woodslee and the alfalfa at Woodslee reduced the soil water status more so than did the lentils at Swift Current.

When the combined impacts of crop rotation with an alternative cultivar were simulated the results mostly emulated the crop rotation approach indicating that the rotational impacts on soil C&N cycling and water storage are of importance (Figs. 6.4-6.6). The impacts on crop growth and N losses were mostly cumulative in effect which is particularly evident at Alfred (Fig. 6.6). The highest SOC storage occurred under this scenario for Woodslee and Alfred, which is not surprising since alfalfa with its dense and deep rooting structure was included in rotation (Fig. 6.7).

6.4 Conclusions and recommendations

In this study we found numerous differences in simulated crop growth and nutrient losses when differing modelling approaches were employed. The differences were generally expected and could be explained based on agronomic principles. Results indicate that every modelling approach considered sometimes influenced model outcomes, depending on the climate, soil, and agronomic system in question. We found at the semi-arid Swift Current location that crop yields were significantly impacted for all approaches except crop rotation. The impact of crop rotation on corn yields and corn silage biomass was, however, strong at the two humid locations. There are observed impacts at Swift Current for other crop rotations such as wheat-canola-wheat-pea which we did not consider in our study (St Luce *et al.,* 2019). Nitrogen losses were generally very low at Swift Current and not strongly impacted by the modelling approaches. An exception was in the case where only min and max temperature and precipitation were used resulting in lower simulated evaporation and greater N leaching below the root zone. The use of fixed fertilizer resulted in greatly increased crop N stress and lower yields in the future under a more favorable climate, however, N loss was only slightly reduced since it was already at minimum levels historically.

At the two humid locations every modeling approach considered resulted in significant impacts on N losses relative to the base approach, either N_2O, N leaching, N runoff or a combination. Fixed fertilizer application showed significant impacts on all three N loss components at the Woodslee location. Reinitialising soils each year and the rotational approach strongly affected soil C&N cycling with clear impacts on N losses. The fixed planting date approach demonstrated low impacts at the humid locations but reduced crop yields by more than 20% in the 2041-2100 time period at Swift Current.

To simulate plausible impacts of climate change on cropping systems we recommend that modellers improve their capabilities of simulating expected changes in agronomy over time and employ tools which consider robust soil-plant-atmospheric processes. We recommend continuous simulation of soil C&N and water cycling over multiple years, use of detailed climate drivers, adjustment of planting dates as climate changes and adjustment of fertilizer rate based on changing SOC mineralization and crop needs. In certain cases crop rotation impacts and influences of possible alternative cultivars should be considered, but there are unlimited possibilities. A model needs to be capable of assessing these impacts but such explorations may be considered adaptation strategies rather than routine modelling methodologies. Note that many of the approaches investigated in this study are commonly employed based on literature. The simple approach with fixed fertilizer, simple climate drivers, and fixed planting is often used in sustainability studies to assess SOC change and N_2O emissions over time. Modelling studies to assess crop growth and development are generally performed using a fuller range of climate drivers but the practice of re-initializing soil status at the start of the growing season is common.

In this study we assessed the impacts of modelling approaches on cropping systems in cool weather conditions. Its expected that the impacts could be large in warmer climates where high heat and water stress are apparent. For instance, if crop yields are negatively impacted under climate change and fixed fertilizer rates are applied then high N losses would be expected. If soils are re-initialized each year the negative influence of reduced C&N and water feedbacks will be ignored and crop growth may be over-estimated. It would be useful to expand and assess modelling approaches under a wider range of climatic conditions globally.

6.5 Supplemental tables and figures

Table 6.S1 Average predicted spring wheat yield, N_2O emissions, N runoff or N leaching for each modelling approach and 30 year time period at the Swift Current location.

Item	Period	Base approach	Minimum climate variables	Fixed fertilizer	Re-initialize soil	Fixed planting	Simple approach	Alternative cultivar	Crop rotation	Cultivar+ crop rotation
Yield	1981-2010	1635Cb[1]	2421Ca	1596Ab	1702BCb	1607Bb	1825Ab	1718Cb	1529Cb	1628Cb
(kg ha^{-1})	2011-2040	1777Cb	2762BCa	1671Ab	1572Cb	1798ABb	1800Ab	2017Cb	1607Cb	1770Cb
	2041-2070	2506Bbc	3276Aa	1968Acd	2110ABcd	1982ABcd	1600Ad	2840Bab	2434Bbc	2520Bbc
	2071-2100	3102Ac	3194ABc	1876Ade	2325Ad	2196Ad	1289Be	3892Aab	3336Abc	4051Aa
N_2O	1981-2010	0.74Bab	0.55Dc	0.82ABa	0.59Cbc	0.74Bab	0.51Cc	0.72Bab	0.66Babc	0.65Bbc
(kg N ha^{-1})	2011-2040	0.69Bab	0.67Cab	0.58Cb	0.77Ba	0.74Ba	0.59Cb	0.72Ba	0.65Bab	0.69Bab
	2041-2070	0.74Babc	0.80Babc	0.68BCc	0.84Ba	0.80Babc	0.70Bbc	0.75Babc	0.76Babc	0.83ABab
	2071-2100	1.05Aabc	1.08Aab	0.86Ac	1.00Aabc	1.14Aa	0.90Abc	1.01Aabc	1.08Aab	0.93Abc
N leaching	1981-2010	0.00Bb	0.99Ba	0.00Bb	0.00Ab	0.00Bb	0.91Ba	0.00Ab	0.00Bb	0.00Bb
(kg N ha^{-1})	2011-2040	0.02Bb	0.91Ba	0.01Bb	0.00Ab	0.01Bb	0.93Ba	0.00Ab	0.00Bb	0.00Bb
	2041-2070	0.19ABb	2.11ABa	0.10ABb	0.01Ab	0.33ABb	1.66ABa	0.00Ab	0.00Bb	0.00Bb
	2071-2100	0.46Ac	3.54Aa	0.26Ac	0.05Ac	0.89Ac	2.53Ab	0.00Ac	0.01Ac	0.00Ac
N runoff	1981-2010	1.57Babc	1.45Bc	1.50Bc	1.46Bc	1.48Bc	1.48Cc	1.54Abc	2.07Ba	2.03Aab
(kg N ha^{-1})	2011-2040	1.74ABab	1.77Bab	1.73ABab	1.57Bb	1.74Bab	1.65BCab	1.46Ab	2.22Ba	1.81Aab
	2041-2070	1.81ABabc	1.94Babc	1.74ABabc	1.85ABabc	1.96Babc	2.07Bab	1.40Ac	2.35Ba	1.56Abc
	2071-2100	2.26Abcd	2.51Abcd	2.13Abc	2.03Ad	2.88Ab	2.84Abc	1.91Ad	3.65Aa	1.88Ad

[1]The uppercase letters represent significant differences between different time periods for the same approach, and lowercase letters represent significant differences between different approaches for the same time period. There are significant differences if letters do not intersect ($p<0.05$).

Table 6.S2 Average predicted corn yield, N_2O emissions, N runoff or N leaching for each modelling approach and 30 year time period at the Woodslee location.

Item	Period	Base approach	Minimum climate variables	Fixed fertilizer	Re-initialize soil	Fixed planting	Simple approach	Alternative cultivar	Crop rotation	Cultivar+ crop rotation
Yield	1981-2010	6023Ab[1]	6548Ab	6053Ab	6049Ab	6023Ab	6480Ab	6023Ab	7272Ba	7275Ca
(kg ha^{-1})	2011-2040	6134Acd	6861Ab	6222Acd	6172Acd	5785Ad	6544Abc	6397Abcd	7800ABa	8153Ba
	2041-2070	6139Ac	6858Ac	6250Ac	6235Ac	6230Ac	6829Ac	6730Ac	7909ABb	8696ABa
	2071-2100	5783Ae	6901Ac	5854Ade	5940Ade	5765Ae	6488Acde	6533Ade	8220Ab	9012Aa
N_2O	1981-2010	7.60Bc	6.99Bc	10.80Ba	7.86Bc	7.88Cc	10.03Cab	7.60Cc	9.02Db	9.04Db
(kg N ha^{-1})	2011-2040	8.53Bbc	7.82Bc	12.02Ba	7.94Bc	9.75Bb	11.90Ba	8.69Bbc	11.04Ca	11.44Ca
	2041-2070	10.40Ad	9.67Ad	14.24Aa	9.77Ad	12.31Ac	14.00Aab	10.63Ad	13.01Bbc	13.69Bab
	2071-2100	11.14Abc	10.32Ac	15.64Aa	10.48Ac	12.34Ab	14.69Aa	11.43Abc	14.67Aa	15.87Aa
N leaching	1981-2010	7.23Babc	8.04ABab	9.10Ba	1.30ABd	6.65Bbc	5.26Bc	7.23Babc	7.44Bab	7.46Bab
(kg N ha^{-1})	2011-2040	6.97Bc	6.26Bc	14.82Aa	1.05Bd	7.69Bc	11.23Ab	7.75Bc	7.11Bc	7.55Bc
	2041-2070	9.48Abc	8.50Ac	13.36Aa	1.78Ad	7.94Bc	7.92Bc	11.34Aab	9.97Abc	11.93Aab
	2071-2100	9.60Acde	7.56ABe	16.45Aa	1.48ABf	11.07Abcd	11.93Abc	13.18Ab	8.56ABde	11.30Abc
N runoff	1981-2010	2.49Cbc	2.39Ccd	3.08Ca	2.19Ad	2.40Ccd	2.68Cb	2.49Cbc	0.76Ae	0.76Ae
(kg N ha^{-1})	2011-2040	2.99Bb	2.95Bb	3.59Ba	2.14Ac	2.85Bb	3.04Bb	2.96Bb	0.77Ad	0.77Ad
	2041-2070	3.41Ab	3.32Ab	4.00Aa	2.37Ac	3.33Ab	3.33Ab	3.45Ab	0.80Ad	0.80Ad
	2071-2100	3.31Ab	3.30Ab	3.98Ab	2.11Ac	3.18Ab	3.30ABb	3.31Ab	0.82Ad	0.82Ad

[1]The uppercase letters represent significant differences between different time periods for the same approach, and lowercase letters represent significant differences between different approaches for the same time period. There are significant differences if letters do not intersect ($p<0.05$).

Table 6.S3 Average predicted silage corn dry biomass, N_2O emissions, N runoff or N leaching for each modelling approach and 30 year time period at the Alfred location.

Item	Period	Base approach	Minimum climate variables	Fixed fertilizer	Re-initialize soil	Fixed planting	Simple approach	Alternative cultivar	Crop rotation	Cultivar+ crop rotation
Biomass	1981-2010	14457Babcd[1]	14128Cd	15213Ba	14082Bd	14304Cbcd	14187Dcd	14466Cabcd	15110Bab	15025Cabc
(kg ha^{-1})	2011-2040	14800Bb	14720Cb	15704Bab	14697Bb	14651Cb	15019Cab	15194Cab	15610Bab	15942Ca
	2041-2070	16777Abc	16344Bbc	16841Abc	16582Abc	16236Bc	16208Bc	17517Bab	17394Aabc	18138Ba
	2071-2100	17469Ac	17256Ac	17039Ac	17258Ac	17258Ac	17000Ac	18987Aab	18238Abc	19588Aa
N_2O	1981-2010	3.55Ccd	3.19Cd	4.54Cab	3.57Ccd	3.71Ccd	4.06Cbc	3.53Ccd	5.11Ca	5.08Ca
(kg N ha^{-1})	2011-2040	3.64Ccd	3.25Cd	4.49Cb	4.07Cbc	4.18Cbc	4.12Cbc	3.71Ccd	5.71Ca	5.78Ca
	2041-2070	4.96Bbc	4.37Bc	5.69Bb	5.67Bb	5.81Bb	5.38Bb	5.10Bbc	7.42Ba	7.73Ba
	2071-2100	6.05Ade	5.49Ad	6.58Acd	7.11Abc	7.58Ab	6.64Abcd	6.30Acde	8.97Aa	9.55Aa
N leaching	1981-2010	11.33Bd	11.93Bd	34.42Ab	20.71Bc	10.90Cd	43.48Aa	11.24Cd	14.48Cd	14.33Cd
(kg N ha^{-1})	2011-2040	14.47Bde	12.72Be	28.23Bb	21.85Bc	15.41ABde	34.28Ba	15.94Bde	17.37BCd	17.82BCd
	2041-2070	14.48Bde	13.24Be	17.24Ccde	23.51Ba	15.12Bde	22.04Cab	17.79Bcd	18.46Bbcd	20.13Babc
	2071-2100	22.30Ac	19.54Ac	18.10Cc	30.52Aab	18.88Ac	18.20Cc	27.99Ab	27.92Ab	32.67Aa
N runoff	1981-2010	1.08Aa	1.06Aa	1.05Aa	1.20Aa	1.09Aa	1.09Aa	1.08Aa	1.14Aa	1.15Aa
(kg N ha^{-1})	2011-2040	0.91Bb	0.91Bb	0.94Ab	1.07ABa	0.92Bb	0.90Bb	0.90Bb	1.14Aa	1.14Aa
	2041-2070	0.80BCe	0.80BCe	0.81Be	1.06Ba	0.78Ce	0.78Ce	0.82BCcd	0.94Bb	0.93Bbc
	2071-2100	0.71Cb	0.69Cb	0.72Bb	0.84Ca	0.67Cb	0.67Cb	0.72Cb	0.92Ba	0.92Ba

[1]The uppercase letters represent significant differences between different time periods for the same approach, and lowercase letters represent significant differences between different approaches for the same time period. There are significant differences if letters do not intersect (p<0.05).

Table 6.S4 Percent difference in spring wheat yield, soil organic carbon, evapotranspiration, N_2O emissions, NO_3^- losses to drains, and NO_3^- runoff between each modelling approach and the base approach at the Swift Current location.

Scenario	1981-2010	2011-2040	2041-2070	2071-2100	1981-2010	2011-2040	2041-2070	2071-2100	1981-2010	2011-2040	2041-2070	2071-2100
	Yield				Soil organic carbon				Evapotranspiration			
Minimum climate variables	48.1	55.4	30.7	3	2.5	5	6.5	5.3	-5.1	-3.9	-9.2	-14.1
Fixed fertilizer	-2.4	-5.9	-21.5	-39.5	0.1	-1.9	-5.5	-12.8	-0.1	-0.2	-0.3	-1.6
Re-initialize soil	4.1	-11.5	-15.8	-25	-0.1	-3.6	-5.9	-10.9	2.8	-1.2	-2	-5.4
Fixed planting	-1.7	1.2	-20.9	-29.2	0.3	1.4	1.9	3.1	0	0.3	0	-0.8
Simple approach	11.6	1.3	-36.2	-58.4	-0.5	-4.5	-8.3	-14.8	-8	-8.5	-14.1	-19.8
Alternative cultivar	5.1	13.5	13.3	25.5	-0.1	0.3	2.9	6.7	1	0.7	1.6	2.5
Crop rotation	-6.5	-9.5	-2.9	7.5	-1.2	-3.2	-5	-6.9	-0.5	-0.7	2.5	7.9
Cultivar + crop rotation	-0.4	-0.4	0.6	30.6	-1	-2.6	-3.1	-2.3	0.7	-1	1.9	8.4
	N_2O				N leaching				N Runoff			
Minimum climate variables	-25.5	-3.1	9	3.6	>100	>100	>100	>100	-7.9	2	7.1	11
Fixed fertilizer	11.4	-15.9	-8.1	-17.8	>100	-20.4	-44.5	-42.9	-4.6	-0.6	-3.6	-5.6
Re-initialize soil	-20.7	11.2	14	-4.4	>100	-100	-94.8	-88.4	-7.2	-9.5	2.2	-10
Fixed planting	-0.6	7.4	8.4	9.5	>100	-70.4	74	95.4	-5.6	0	8.4	27.3
Simple approach	-31.5	-14.3	-5.5	-14	>100	>100	>100	>100	-6.1	-5.1	14.7	25.7
Alternative cultivar	-2.5	4	2	-3	>100	-100	-100	-99.6	-2.1	-15.7	-22.8	-15.5
Crop rotation	-10.6	-5.5	3.3	3	>100	-100	-100	-100	31.5	27.7	29.9	61.5
Cultivar + crop rotation	-11.9	0.3	12.6	-10.6	>100	-100	-100	-100	29	4.2	-13.9	-16.6

Table 6 S5 Percent difference in grain corn yield, soil organic carbon, evapotranspiration, N_2O emissions, NO_3^- losses to drains, and NO_3^- runoff between each modelling approach and the base approach at the Woodslee location.

Scenario	1981-2010	2011-2040	2041-2070	2071-2100	1981-2010	2011-2040	2041-2070	2071-2100	1981-2010	2011-2040	2041-2070	2071-2100
	Yield				Soil organic carbon				Evapotranspiration			
Minimum climate variables	8.7	11.8	11.7	19.3	1.1	2.7	3.5	4.4	-11.3	-12.5	-13.3	-11.7
Fixed fertilizer	0.5	1.4	1.8	1.2	0.2	0.8	1.6	1.5	0.1	0.1	0.1	0.1
Re-initialize soil	0.4	0.6	1.6	2.7	-3.7	-6.6	-7.5	-8.3	0.3	-0.7	-1.4	-1.7
Fixed planting	0	-5.7	1.5	-0.3	1.1	0.2	0.6	0.1	-0.2	-0.2	1.8	1.7
Simple approach	7.6	6.7	11.2	12.2	1.6	2.4	3.1	3.2	-11.3	-12.1	-11.6	-10.8
Alternative cultivar	0	4.3	9.6	13	0	0.8	2.3	3.4	0	0.9	1.6	2.1
Crop rotation	20.6	27.2	29.2	42.3	3.8	11.8	18.3	24.8	7.4	8.3	7.8	8.6
Cultivar + crop rotation	20.7	32.9	42.2	56.1	3.9	12.3	19.9	27.6	7.4	9.8	10.3	10.9
	N_2O				N leaching				N Runoff			
Minimum climate variables	-8	-8.3	-7	-7.3	11.3	-10.3	-10.3	-21.2	-3.7	-1.5	-2.8	-0.5
Fixed fertilizer	42	40.9	36.9	40.4	25.8	112.6	41	71.4	23.7	19.9	17	20.1
Re-initialize soil	3.4	-6.9	-6.1	-5.9	-82	-84.9	-81.2	-84.5	-12.1	-28.4	-30.7	-36.3
Fixed planting	3.6	14.3	18.4	10.8	-8	10.4	-16.2	15.3	-3.4	-4.9	-2.5	-4
Simple approach	31.9	39.5	34.7	31.9	-27.2	61.2	-16.4	18.7	7.7	1.6	-2.4	-0.3
Alternative cultivar	0	1.9	2.2	2.6	0	11.2	19.7	37.4	0	-1.3	1.2	-0.1
Crop rotation	18.5	29	25.6	31.6	2.4	2	5.1	-11.4	-69	-74.4	-76.3	-75
Cultivar + crop rotation	18.7	33.8	32	42.4	2.7	8.4	25.6	16.8	-69	-74.5	-76.5	-75.1

Table 6.S6 Percent difference in silage corn biomass, soil organic carbon, evapotranspiration, N_2O emissions, NO_3^- losses to drains, and NO_3^- runoff between each modelling approach and the base approach at the Alfred location.

Scenario	1981-2010	2011-2040	2041-2070	2071-2100	1981-2010	2011-2040	2041-2070	2071-2100	1981-2010	2011-2040	2041-2070	2071-2100
	Yield				Soil organic carbon				Evapotranspiration			
Minimum climate variables	-2.9	-0.5	-2.6	-1.2	-0.1	0.4	0.6	0.9	-12.5	-12.1	-12.9	-12.7
Fixed fertilizer	4.5	6.1	0.4	-2.5	1.3	2.5	1.9	0.8	0.8	0.9	0	0
Re-initialize soil	-3.3	-0.7	-1.2	-1.2	1.5	3.5	3.8	4.8	-1.1	-0.8	-0.9	-1.5
Fixed planting	-1.7	-1	-3.2	-0.7	0	-0.1	-0.3	0.1	-0.2	0.5	-0.6	0.3
Simple approach	-2.5	1.5	-3.4	-2.7	0.6	1.7	1.9	2	-12.3	-11.7	-12.9	-12.3
Alternative cultivar	-0.6	2.7	4.4	8.7	-0.1	0.3	0.9	2.3	-0.1	0.9	1.3	2.2
Crop rotation	3.9	5.6	3.5	4.6	2.7	6.7	8.7	11.4	2	1.8	1.3	1.3
Cultivar + crop rotation	3.3	7.8	7.9	12.4	2.7	6.8	9.2	12.6	1.8	2.6	2.8	3.7
	N_2O				N leaching				N Runoff			
Minimum climate variables	-10	-10.6	-11.9	-9.3	5.4	-12.1	-8.6	-12.4	-1.9	0.7	0.1	-2.5
Fixed fertilizer	28	23.4	14.7	8.8	203.9	95.1	19.1	-18.8	-3.1	3.8	0.5	1.7
Re-initialize soil	0.6	12	13.7	17.6	82.9	51	62.3	36.9	11.2	18.3	32.5	18.4
Fixed planting	4.5	14.9	17.1	25.3	-3.7	6.5	4.4	-15.3	0.8	1.1	-2.4	-5
Simple approach	14.5	13.3	8.4	9.9	283.9	136.9	52.2	-18.4	0.8	-0.4	-2.8	-5.9
Alternative cultivar	-0.4	2.1	2.9	4.3	-0.8	10.2	22.8	25.5	-0.2	-1.2	1.9	0.9
Crop rotation	44.3	56.8	50.5	48.1	28	19.1	28.3	24.6	5.5	25.1	16.8	28.9
Cultivar + crop rotation	43.4	58.9	56.6	57.6	26.7	22.3	40	45.8	5.4	26.6	15.8	29.1

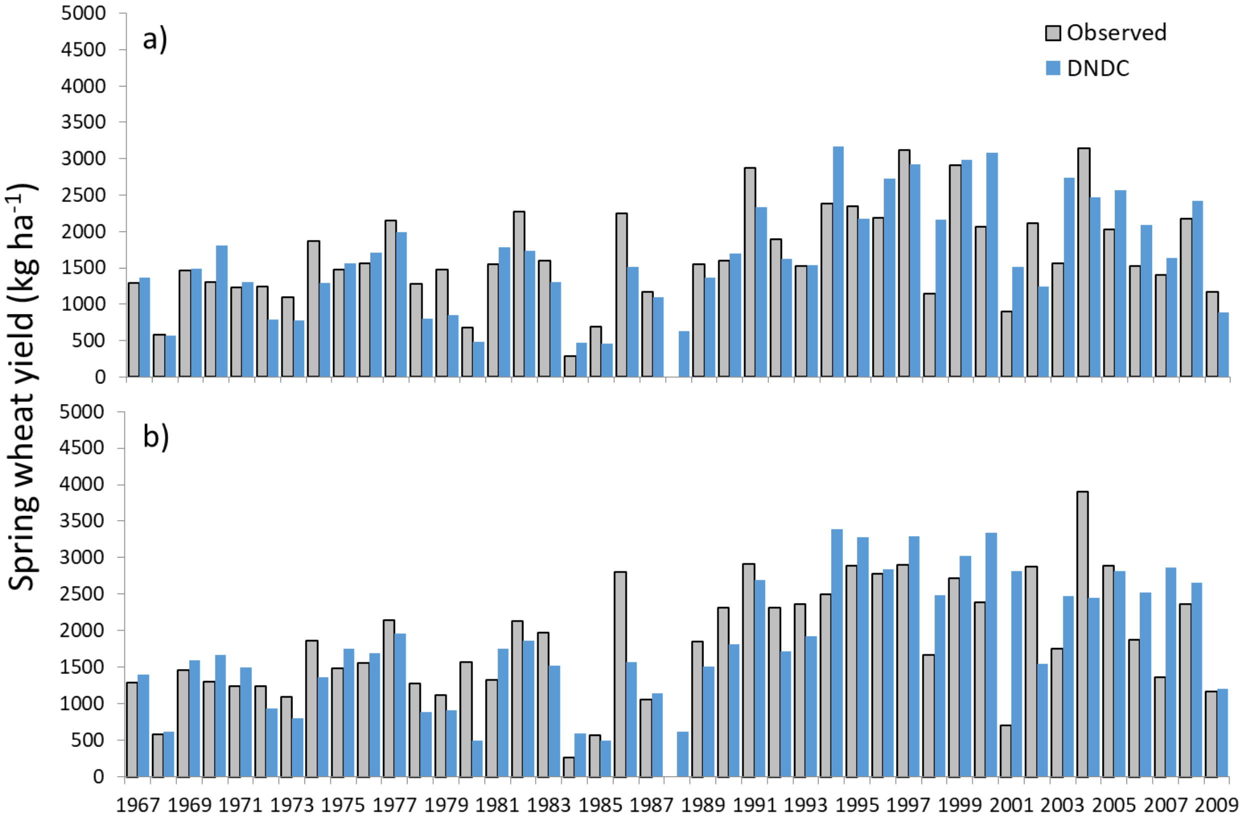

Figure 6.S1 Comparison of observed and simulated grain yields for a) monoculture spring wheat and b) rotational spring wheat in a spring wheat-lentil rotation at the Swift Current location.

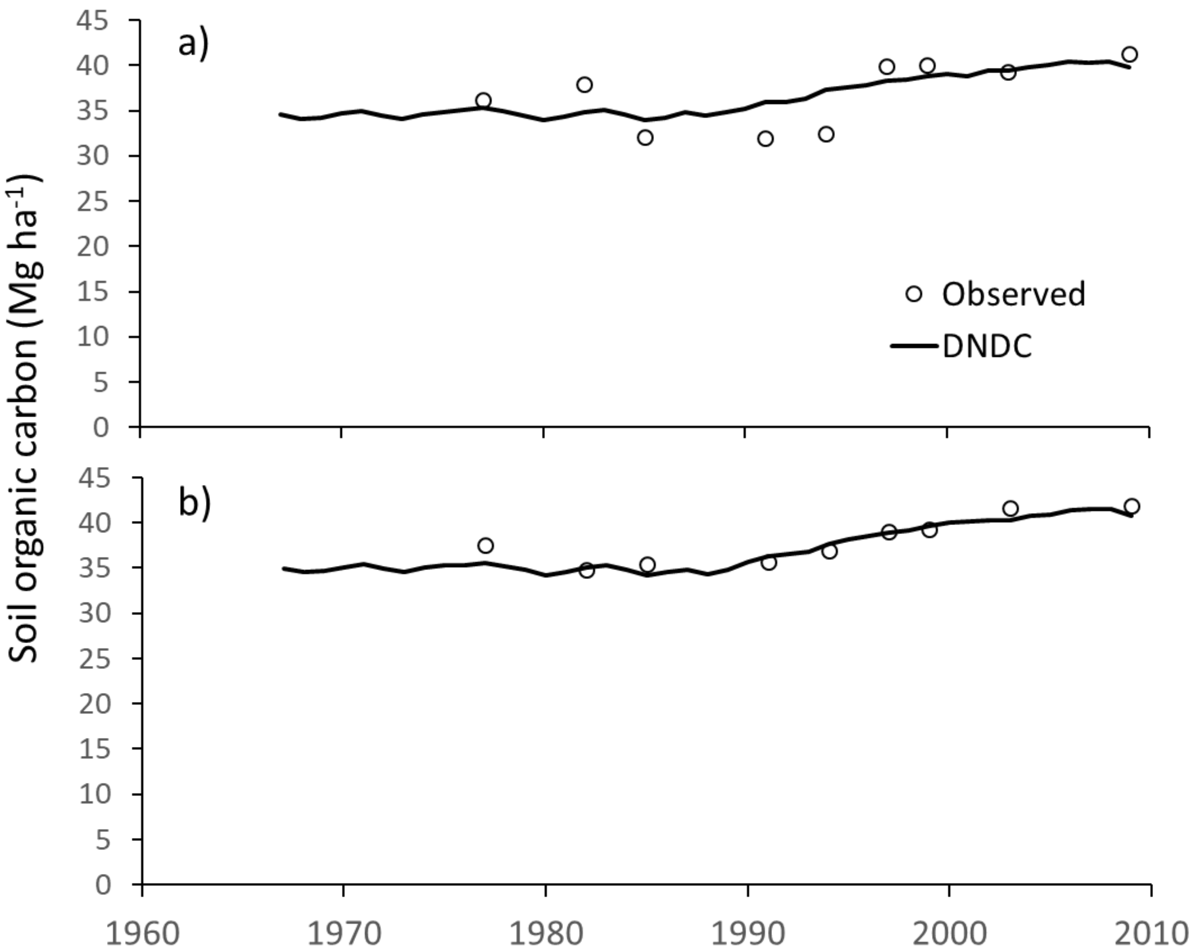

Figure 6.S2 Observed and simulated soil organic carbon from 0-15 cm depth for a) monoculture spring wheat and b) rotational spring wheat-lentil at the Swift Current location

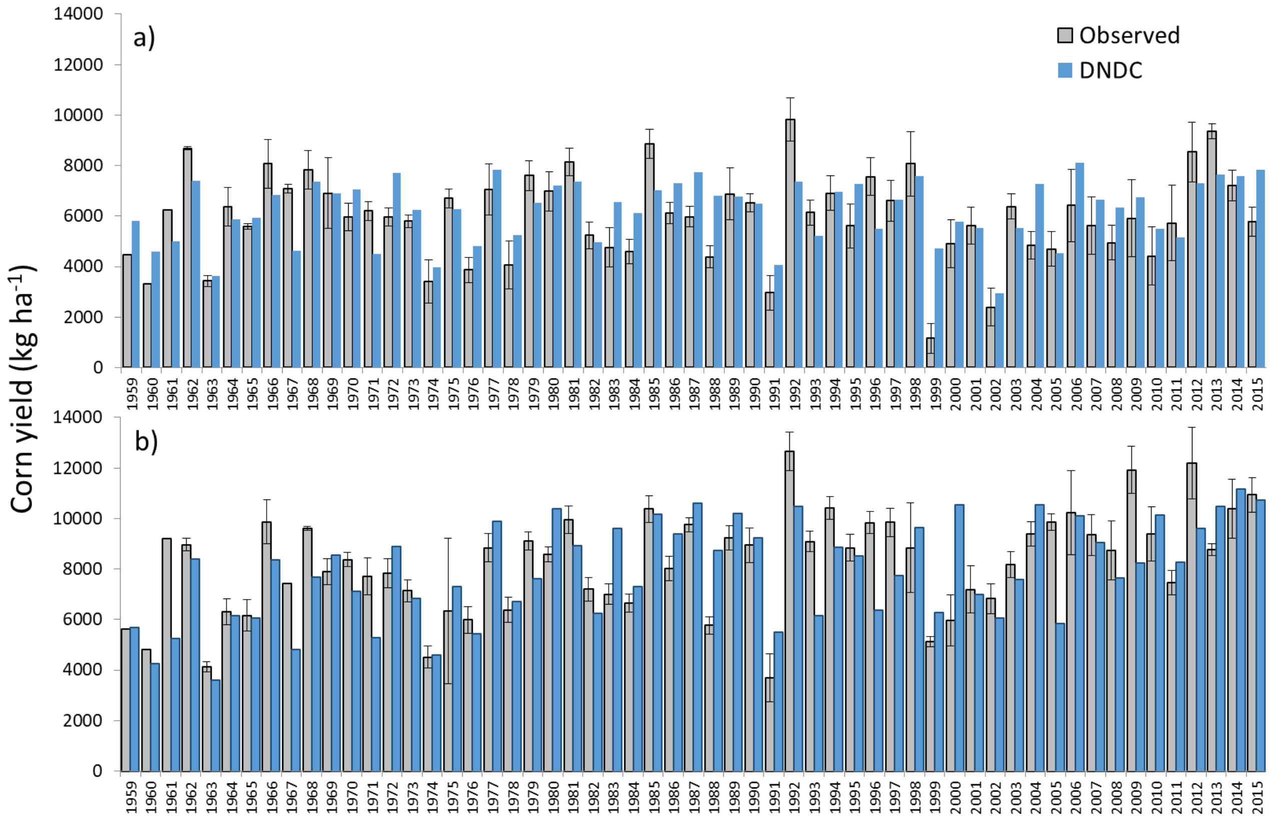

Figure 6.S3 Comparison of observed and simulated grain yields for a) monoculture corn and b) rotational corn in a corn-oats-alflalfa-alfalfa rotation at the Woodslee location.

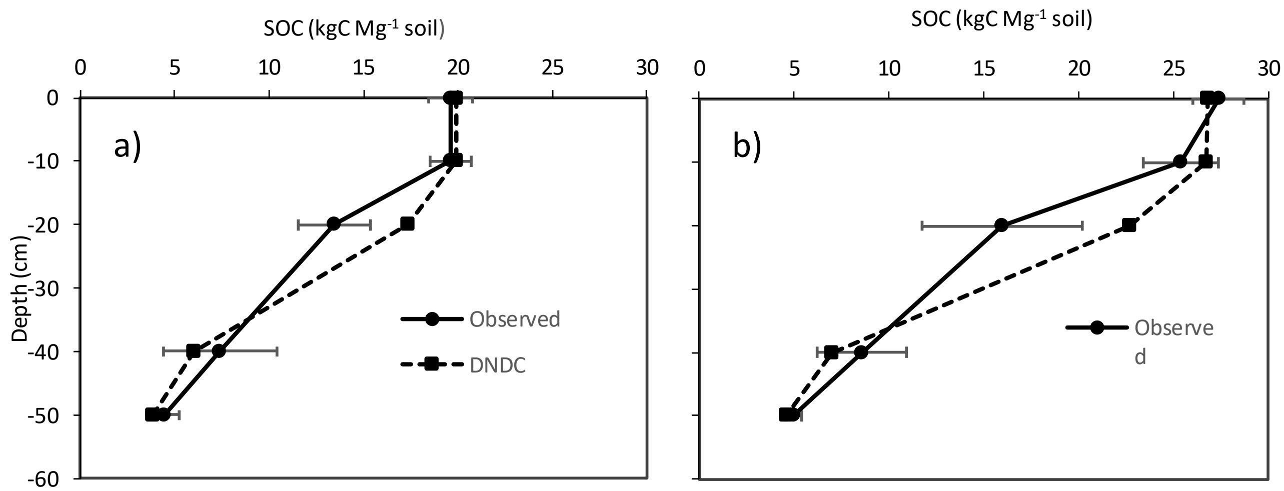

Figure 6.S4 Observed and simulated SOC in the soil profile at Woodslee for a) the continuous corn rotation and b) the corn-oats-alflalfa-alfalfa rotation. SOC is averaged from 2004-2007, 46 years after the implementation of the long-term trial.

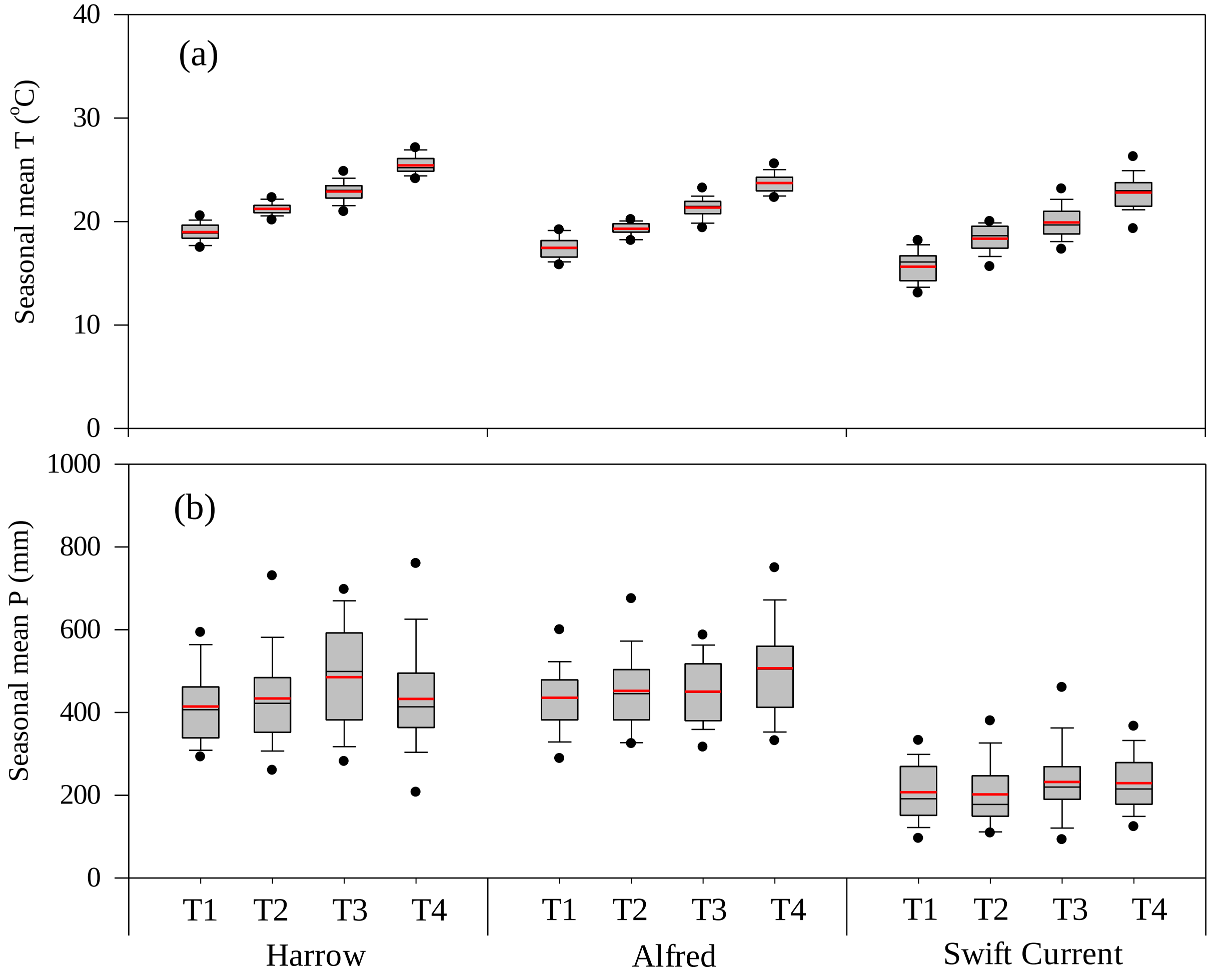

Figure 6.S5 Growing season average temperature and precipitation under the 8.5 Watt m^{-2} climate change scenario. The growing season is calculated from May 1st to August 31st for spring wheat (Swift Current) and from May 1st to September 30th for corn (Harrow) and silage corn (Alfred). T1, T2, T3 and T4 represent the time periods 1981-2010, 2011-2040, 2041-2070, and 2071-2100, respectively

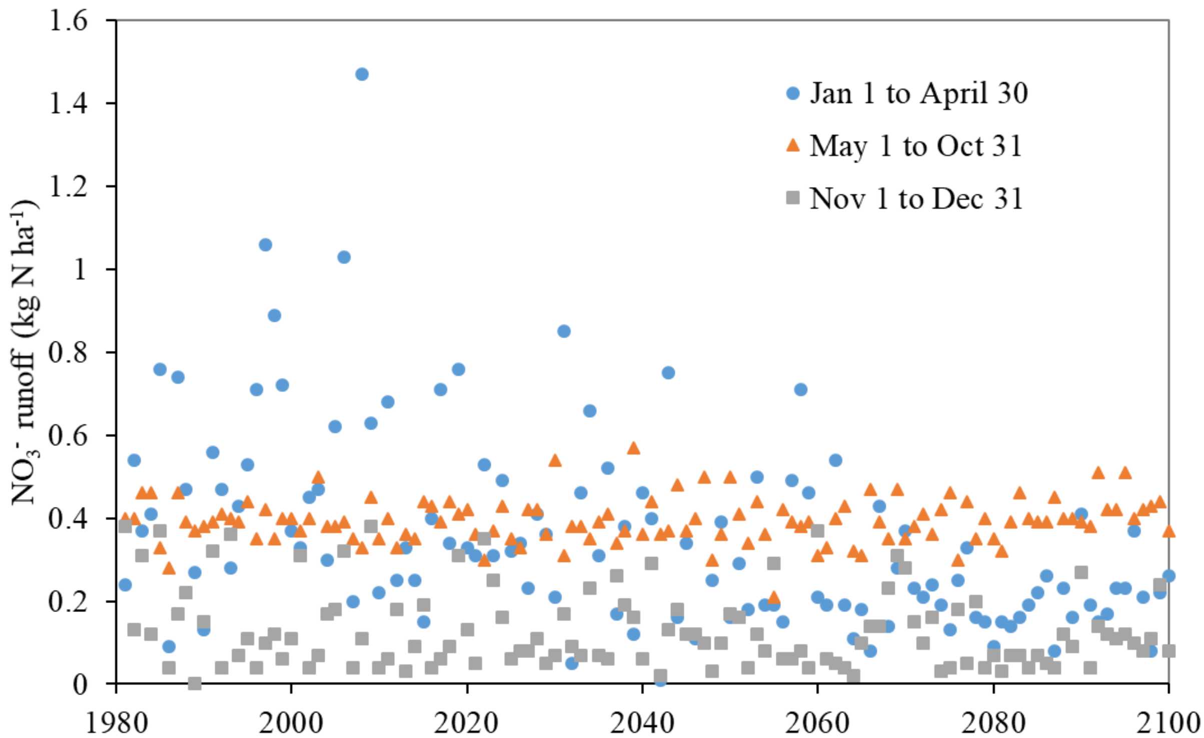

Figure 6.S6 Simulated NO_3^- runoff for the base modelling approach in the early, mid and late season at Alfred.

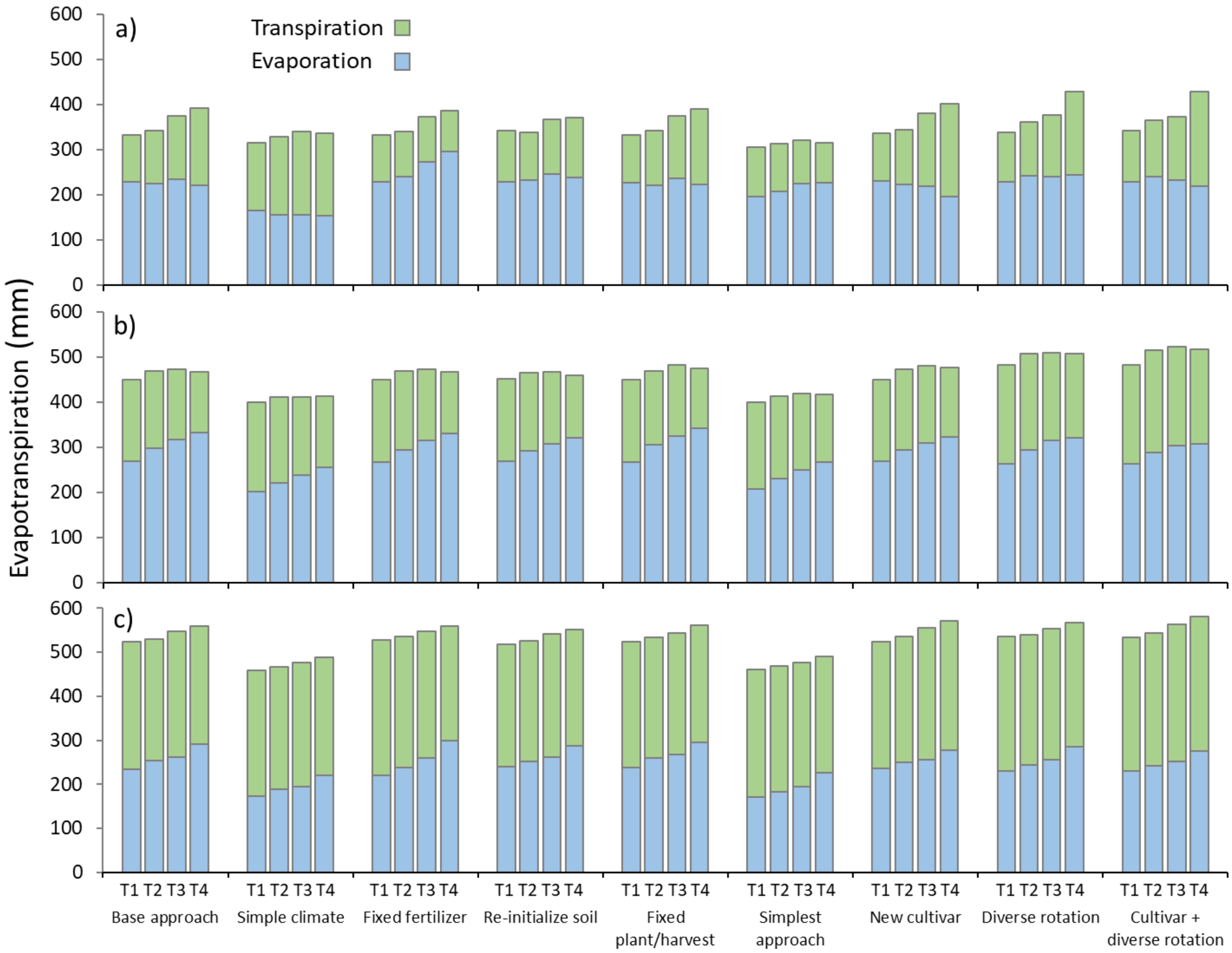

Figure 6.S7 Average simulated evaporation and transpiration for each modelling approach at the a) Swift Current, b) Woodslee and c) Alfred locations across each 30 year time period. T1, T2, T3 and T4 represent the time periods 1981-2010, 2011-2040, 2041-2070.

Chapter 7

Summary and conclusions

7.1 General overview

The main goal set out in this thesis was to improve the ability of the DNDC model for simulating soil hydrology, partly by incorporating a new drainage sub-model, to advance its capacity for assessing the sustainability of cropping systems, both under current and future climate. The model was successfully expanded to simulate soil hydrology and N losses with similar accuracy as the RZWQM2, while minimizing the computation time, input requirements, and the level of expertise required to operate the model. The revised model can now simulate the impacts of tile drainage depth and spacing, controlled drainage and sub-irrigation on crop growth and development and soil C&N and water cycling. Application of the revised model, which could better simulate interactions between environmental outcomes, was then demonstrated by exploring reactive N losses for 18 fertilizer management scenarios at three research sites and by formulating a recommended modelling approach for simulating the impacts of climate change on cropping systems.

7.2 Conclusions

Objective 1: To compare the performance of the default DNDC model, which utilizes simplified expressions for water dynamics to the more hydrologically complex RZWQM2 using a detailed dataset of crop biomass and N uptake, soil water content, drainage, and N loading to tiles. Recommend improvements to DNDC.

A study was implemented to compare the performance of two widely used process-based models for simulating crop growth and soil water dynamics and N loss to tile drains. It was informative to discover that a simple cascade water sub-model (DNDC) performed adequately in comparison to measurements and similarly with respect to RZWQM2 across certain metrics including crop yield, biomass, N uptake of winter rye, annual and monthly water flow and N loss to tile drains. There were, however, shortcomings in simulating soil water storage, soil water contents down the profile and daily water flow events whereas RZWQM2 generally performed adequately for these metrics. Fine scale temporal simulation of water and N dynamics can greatly impact soil water and nutrient levels, thereby influencing several biogeochemical processes such as decomposition, denitrification, nitrification and methanogenisis. These processes are largely dependent on soil water content. Since DNDC is primarily used to simulate GHG emissions we recommended that developments be carried out for DNDC to further improve its hydrological processes.

Suggested improvements for DNDC included a deeper and heterogeneous soil profile, inclusion of root distribution functions, inclusion of improved water flow, a fluctuating water table, and a new tile drainage sub-model. Considerations should, however, be taken when contemplating model developments. More complex processes can increase model input requirements, computation time and the required level of modeller expertise.

Objective 2: To revise hydrologic processes in the DNDC model by including a new tile drainage sub-model, ability to simulate controlled drainage and sub-irrigation, improved soil water flow, a heterogeneous soil profile, revised root penetration and density functions, and a deeper soil profile. Compare the performance of the revised DNDC model to RZWQM2 using detailed datasets of runoff and drainage in eastern Canada and the US Midwest.

To improve the performance of the DNDC model for simulating soil hydrology we implemented a deeper and heterogeneous soil profile, root penetration and density functions, a fluctuating water table, unsaturated flow above field capacity, and the Hooghoudt equation to simulate mechanistic tile drainage based on drain spacing, depth and tile diameter. After development, simulations of soil water storage, daily drainage, N loss to runoff and N loss to tile drains were improved, comparing well to measurements at two research sites and showing at least as good of performance as RZWQM2. This demonstrated that DNDC development was successful considering RZWQM2 is a well-validated water quality model which includes detailed computational hydrology. The soil-water input requirements for DNDC were kept relatively low and the model simulation time remained four times faster than RZWQM2, which are important factors for larger scale assessments. Neither the revised DNDC model or RZWQM2 well simulated the timing of water or N losses to runoff but performed satisfactory in simulating the cumulative magnitudes. The simulation of runoff is complex particularly when surface crusting, clay cracking, preferential flow through insect and root channels, snow dynamics, and soil freeze-thaw are prevalent and further research is recommended. DNDC was able to capture the observed differences in water and N losses between conventional drainage and controlled drainage management with sub-irrigation.

Through these developments we expanded the ability of DNDC to simulate the impacts of tile drainage management on several biogeochemical processes. Future studies can now investigate optimum tile drain depth and spacing, and explore possible benefits of controlled drainage or sub-irrigation on crop growth, soil C&N cycling and reactive N losses.

Objective 3: To use the revised DNDC model to investigate inorganic and organic fertilizer management practices over a 30 year time horizon to determine practices which may reduce reactive N loss from corn silage production in cool climatic zones of eastern Canada and the US Midwest. and to examine trade-offs and synergies between N loss to tile drains, N loss to runoff, NH_3 volatilization and N_2O emissions. Recommend beneficial management.

The revised and well-tested DNDC model was used to investigate the impacts of N loss from 18 fertilizer management practices across 3 locations, fine and coarse soil textures at each location, and 30 years of climate variability. Management scenarios included fertilizer type (manure slurry and urea fertilizer), timing (spring, fall, split, side-dress) and method of application (injected, incorporated, broadcast). Reactive N losses (N to drainage and runoff, N_2O and NH_3) were greatest from broadcast, followed by incorporated and then injected. The inputs for the DNDC model were constructed using R statistical software (R Core Team, 2013) to build 3240 iterative permutations of climate and management and soil type.

Similar impacts of fertilizer management were often determined between locations and these were highly variable across climate but usually agreed with observations. Reactive N losses were much greater from coarser than the finer textured soils and in many cases climate variability had more influence on reactive N loss than did changes in fertilizer management. More NH_3 volatilization and N_2O losses occurred from organic fertilizer but N leaching was similar. There was, however, much greater N leaching and runoff from fall applied than spring applied manure slurry. The most beneficial managements were shown to be split and side-dress mineral fertilizer. Ranking of reactive N losses across the 18 fertilizer management practices were provided in the manuscript for each location and soil type.

Several on farm management decisions come into play when considering fertilizer application method. These can include fertilizer source and type of equipment available for application, manure storage considerations, and on farm time management between multiple tasks. The results presented in this study can be used to guide producers in planning fertilizer management in an effort to reduce N loss, and minimize the environmental footprint.

Objective 4: To investigate the implications of using simpler versus more advanced modelling approaches for simulating the impacts of climate change on crop production, SOC change, N_2O emissions and N leaching and runoff and recommend an approach under cool weather climates. Assess the effect of climate change on crop production and sustainability for common cropping systems in Canada.

Well developed and calibrated biophysical models can be particularly valuable for simulating climate change impacts, however, there are many alternative modelling approaches used in literature for simulating such impacts. These approaches usually employ simplified methods to avoid complexities that some crop-focused models cannot handle, such as long-term feedbacks in soil C&N and water cycling over time. We performed case studies at three locations in Canada to explore the impact of modelling approaches that are commonly employed in literature which may adversely impact the simulation of crop yields, soil organic carbon change and N losses. These included the use of a minimum set of weather variables, re-initializing soil status annually, fixed fertilizer application rates, fixed planting dates, and ignoring changes in crop cultivars and rotational impacts. The approaches were compared to a comprehensive base approach where detailed climate drivers, adjustment of planting dates, fertilizer rates based on crop needs, and continuous simulation of soil C&N and water feedbacks were considered.

We found numerous differences in simulated crop growth and nutrient losses when differing modelling approaches were employed. The differences were generally expected and could be explained based on agronomic principles. Results indicated that every modelling approach considered, with respect to the base approach, sometimes influenced model outcomes, depending on the climate, soil, and agronomic system in question. We found at the semi-arid Swift Current location that crop yields were significantly impacted for all approaches except crop rotation. At the two humid locations every modeling approach considered resulted in significant impacts on N losses relative to the base approach, either N_2O, N leaching, N runoff or a combination. Fixed fertilizer application showed significant impacts on all three N loss components at the Woodslee location. Reinitialising soils each year and the rotational approach strongly affected soil C&N cycling with clear impacts on N losses. The fixed planting date approach demonstrated low impacts at the humid locations but reduced crop yields by more than 20% in the 2041-2100 time period at Swift Current.

To simulate plausible impacts of climate change on cropping systems we recommend that modellers improve their capabilities of simulating expected changes in agronomy over time and employ tools which consider robust soil-plant-atmospheric processes. We recommend continuous simulation of soil C&N and water cycling over multiple years, use of detailed climate drivers, adjustment of planting dates as climate changes and adjustment of fertilizer rate based on changing SOC mineralization and crop needs. In certain cases crop rotation impacts and influences of possible alternative cultivars should be considered as adaptation measures.

7.3 Contributions to knowledge

The research performed in this thesis resulted in several contributions which fill gaps in knowledge within the international modelling community. The study which compared hydrological model frameworks was not only useful for understanding issues that occur in the DNDC model but it has implications for many well-known agricultural models that use a cascade flow approach. To accurately estimate daily water and N losses to tile drains and soil water storage in cropping systems the simulation of soil hydrology requires improvement in many of these models.

The development of a revised DNDC model for simulating soil hydrology and the inclusion of a new tile drainage sub-model is a significant contribution to the agricultural modelling community, especially since the reasons for implementing specific components are well documented. The model can for the first time simulate the impacts of drainage depth and spacing, controlled drainage and sub-irrigation thus it can now estimate drainage design impacts on GHG emissions, NH_3 volatilization, N losses to tiles and runoff, and SOC dynamics. The DNDC.vCAN model is currently being used by at least a dozen modelling groups worldwide with an increasing user base trend. There is considerable interest in using the revised hydrology version. Now that hydrology has been improved, the model can be further improved for simulating several biogeochemical processes and can be used as a science-based research tool to investigate BMPs and climate change impacts on cropping systems. The revised model, being able to simulate a wider range of sustainability metrics, will be integrated into a number of research programs within Agriculture and Agri-Food Canada.

The investigation of fertilizer management decisions across a long-term climate horizon in this thesis serves as a guide for producers in planning fertilizer management in an effort to reduce N loss, maintain crop productivity and minimize the overall environmental footprint of farming activities. This study serves as an example of how a well evaluated process-based model can be applied to assess the trade-offs in a number of environmental outcomes, rather than focusing on only one metric (such as crop yield, GHG emissions, or water quality). The model automation procedure developed in this study is currently being employed for several other projects.

The manuscript on assessing modelling approaches for simulating climate change impacts on cropping systems should serve as a valuable guide and reference for many future modelling studies. Many of the simpler modelling methods investigated are shown to produce results that are not plausible, however, such methods are commonly employed by modellers worldwide. The simulations using our revised DNDC model clearly document deficiencies in many of these approaches and its likely that the recommendations we put forth will help guide the modelling community to use improved methodologies.

7.4 Recommendations for future research

The poor simulation of soil hydrology in the DNDC model adversely impacted the simulation of several processes. Now that the model has been improved several processes can be re-evaluated as follows:

1. Focus can now be placed on improving biochemical processes that impact N_2O emissions. In several studies it was found that DNDC underestimated N_2O emissions during periods of high rainfall or spring snow melt due to the inability of a cascade flow model to simulate water contents above field capacity. Soil water strongly influences oxygen diffusion into the soil and the type of denitrification reactions that occurs. Datasets can now be used to properly update this process by setting the range of N_2O production in the model to occur an appropriate soil water and oxygen content range. Further, the DNDC model does not separately characterize N_2O production and consumption processes, and diffusion is only handled in a simplistic empirical manner. Soil water content and substrate availability (N in solution) are important drivers of these

processes thus advancements may be made now that soil water and N simulation have been improved.

2. DNDC simulates the impact of urease and nitrification inhibitors on N cycling, relevant to NH_3 volatilization, N_2O emissions, and N leaching and runoff. However, the implementation of inhibitor simulation requires improvement to allow for non-linear efficiencies of the inhibitors. Also the leaching characteristics of urea should be improved, since this strongly impacts the function of the inhibitors.
3. The simulation of runoff including N and P lost via runoff is complex particularly when surface crusting, clay cracking, preferential flow through insect and root channels, snow dynamics, and soil freeze-thaw are prevalent and further research to improve DNDC is recommended. Very good data sets are required which characterize not only runoff but also the extent and depth of clay cracking and crusting, *in situ* measured hydraulic conductivities, soil water tension and snow depth and density.
4. The capability to simulate phosphorous dynamics is available in DNDC, however, the functions are rarely applied or tested against measured data. Phosphorous losses through runoff from agroecosystems are of course very important contributions to eutrophication of water bodies thus this warrants testing and possible developments.
5. The model has been extended to 2m simulation and a fluctuating water table with quasi-2D tile drainage has been incorporated. This has positive implications on the simulation of SOC dynamics. The simulated impacts of tile drainage design on SOC storage, including subsurface drainage and sub-irrigation, can now be evaluated and the model can be applied to identify BMPs. Further, buried SOC occurs particularly in eastern North America and Europe, in more humid regions where mouldboard ploughing is used. Over time, a portion of the crop residues is turned over and buried below the plough layer where it remains more stable. This is seldom simulated in agricultural models but is deemed important since models do not simulate the correct total balance of SOC in the profile. The simulation of a buried SOC should now be implemented in DNDC.
6. Most agricultural models including DNDC do not include the impacts of plant disease and pests. However, many stand-alone empirical models are available which include these impacts and they could be incorporated into DNDC. The drivers of plant disease such as relative humidity, soil water content, canopy temperature, and radiation are

already included in the model thus the incorporation of these empirical-based models is a good opportunity, particularly since the simulation of certain drivers has been improved.

In this thesis the revised DNDC model has been successfully calibrated and validated and used to investigate management impacts on several metrics under climate variability and climate change. Simulations can now be extended for more extensive applications as follows:

7. It's important that the DNDC model be evaluated for additional cropping systems in Canada and worldwide. Much can be learned regarding the simulation of crop growth and development, hydrologic systems modelling, and soil C&N cycling under the scope of the Agricultural Model Intercomparison and Improvement Project (AgMIP) and the Global Research Alliance (GRA) Integrative Research Group.
8. The model automation infrastructure developed in Chapter 5 could be employed to estimate trade-offs in nutrient losses for a wider range of crop types, management activities and locations. The model can now generate more reliable and a wider range of sustainability metrics which could be useful for improving the Canadian GHG and soil carbon inventories and the National Agri-environmental Indictors.
9. Now that we have defined an approach for simulating climate change impacts (Chapter 6) studies can be implemented which model the resilience and sustainability of a wide range of agricultural management practices under future climates. It is generally expected that N losses will increase in the future but diversified crop rotations, improved drainage and irrigation, tillage or residue management may mitigate these losses. There is interest in determining how climate change will impact crop water use and nitrogen fertilizer application rates in the future and how cropping patterns might change in existing agricultural regions, or which regions may open up for annual cropping (such as the northern clay belt in Ontario).
10. There are opportunities to link the DNDC model with a Life Cycle Analysis (LCA) tool to estimate the global warming potential, acidification or eutrophication of agricultural products at the farm gate. A well evaluated biogeochemical model can provide improved estimates of GHG emissions, NH_3 volatilization and water quality that are needed for a quality analysis. An LCA tool such as the one developed by Goglio et al. (2018) could be

coupled within the DNDC interface to enable the estimation of emissions and energy from farm machinery, as well as upstream processes of fertilizer and pesticide production, etc. Likewise, an economic assessment of cropping systems could be linked using current crop sales data, machinery and labour costs. For Canada, this data is available from within the Canadian Regional Agricultural Model (CRAM) developed and used by Strategic Policy Branch of Agriculture and Agri-Food Canada.

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