Mitigating Greenhouse Gas Emissions in Subsurface-Drained Fields in Eastern Canada

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Abstract

In wet regions subsurface drainage is essential in removing excess water in soil and promoting crop growth; however, it may also result in environmental problems. Implementation of agricultural best management practices (BMPs) on subsurface-drained lands can mitigate environmental problems brought on by human activities and climate change. To provide effective mitigation and adaptation measures for the management of subsurface-drained fields, a quantitative assessment of the impact of water table depth, agronomic management practices, and climate-change-driven rises in greenhouse gas (GHG) emissions on water quality and crop production were assessed through an modeling approach (Root Zone Water Quality Model, RZWQM2).

Drawing on a comprehensive hydrological dataset (*i.e.*, tile drainage, sub-irrigation, soil water content, sap flow and crop growth) for calibration, the RZWQM2 then accurately simulated crop growth and growing season drainage. However, the model significantly overestimated winter tile flow, indicating its reliability to be compromised by its imperfect winter drainage process. Implementation of Kalman filter technique successfully enhanced model reliability and reduced predictive uncertainties in simulating winter drainage in cold areas. The revised modelling approach could then serve to evaluate water and field management scenarios for subsurface-drained and irrigated fields.

A comparison of the abilities of the RZWQM2 and DNDC models to comprehensively simulate both crop growth and the biogeochemical processes occurring within the soil profile, showed both models to accurately estimate soil temperature, but DNDC to perform poorly in

simulating the soil water content (SWC) due to the lack of a heterogeneous soil profile, shallow simulation depth and lack of root density functions for crops. Both models showed similar performances in simulating N_2O emissions, with predicted cumulative N_2O emissions being with ±15% of measured vales for all four treatments; however, RZWQM2 better estimated CO_2 emissions (greater R^2, lesser root mean square error). Both models accurately (within ±15%) estimated cumulative growing season drainage; however, RZWQM2 was more accurate in predicting daily drainage and DNDC was not equipped to simulate controlled drainage or sub-irrigation. Both models performed satisfactorily in predicting grain yields of corn and soybean. Overall, RZWQM2 proved to be more applicable to simulating the biogeochemical processes in sub-surface drained fields than DNDC.

RZWQM2 was used to evaluate different potential BMP's ability to mitigate GHG emissions in a subsurface-drained corn (*Zea mays* L.) field under water table management. The optimal range of N fertilization to reduce GHG emissions while maintaining high nitrogen use efficiency and crop yields was identified as 125 to 175 kg N ha^{-1}. Splitting N applications was found to reduce total N_2O emissions by 11%. Controlled drainage with subirrigation resulted in 21% greater N_2O emissions, but 6% lower CO_2 emissions compared to free drainage. A corn-soybean rotation reduced GHG emissions by 20% over continuous corn.

Climate change impacts on crop production, water quality and GHG emissions from subsurface drained fields at two sites of Eastern Canada were assessed using RZWQM2. Under future climate scenarios, mean drain flow and N losses through drainage would increase by 23-41% and 47-76%, respectively. The N_2O emissions would rise by 21-25% due to greater denitrification and mineralization, while CO_2 emissions would rise by 16% due to greater crop biomass accumulation, faster crop residue decomposition, and greater soil microbial activity.

These simulations further indicated that future corn yields would decline, while soybean yields would increase in the future, and that climate change would exacerbate environmental pollution by increasing the GHG emissions from croplands and N losses in drainage.

Résumé

Dans les régions humides le drainage souterrain s'avère essentiel a l'évacuation de l'excès d'eau dans le sol et à promouvoir la croissance des cultures; cependant, il peut aussi causer des problèmes environnementaux. La mise en œuvre de meilleures pratiques de gestion (MPGs) sur les terrains agricoles équipés d'un réseau de drainage souterrain peut permettre de mitiger les problèmes environnementaux advenant d'activités humaines et du changement climatique. Afin d'offrir des mesures efficaces de mitige et d'adaptation pour la gestion des terrains agricoles équipés d'un réseau de drainage souterrain, une technique de modélisation (Root Zone Water Quality Model, RZWQM2) fut appliquée à l'évaluation quantitative de l'impacte du niveau de la nappe phréatique, des pratiques de gestion agronomiques et de la hausse des émissions de gaz à effet de serre (GES) liée au changement climatique, sur la qualité de l'eau et la production agricole. Puisant dans une base de données hydrologique exhaustive (c. à d., drainage souterrain, irrigation souterraine, humidité du sol, écoulement de la sève, et croissance de la culture) lors de l'étalonnage du modèle, RZWQM2 simula alors fidèlement la croissance de la culture et le volume saisonnier des eaux de drainage. Cependant, le modèle largement surestima l'écoulement hivernal par drains souterrains, compromettant ainsi la fiabilité de son processus de simulation du drainage hivernal. La mise en œuvre d'une méthodologie avec filtre de Kalman améliora la fiabilité du modèle, réduisant ainsi la marge d'incertitude de la simulation des eaux de drainage souterrains hivernaux dans les régions froides. Le modèle RZWQM2 amélioré pouvait donc servir à l'évaluation de scénarios de gestions des eaux et des terres agricoles pour les champs irrigués et dotés d'un système de drainage souterrain.

Une comparaison de la capacité des modèles RZWQM2 et DNDC à simuler d'une façon exhaustive à la fois la croissance des cultures et les processus biogéochimiques ayant lieu à travers le profil du sol, montra que les deux modèles donnèrent une estimation exacte de la

température du sol, mais que, n'étant ni capable de simuler un profil du sol profond ou hétérogène, ni la masse volumique de racines de la culture, DNDC fut peu performant quant à la simulation de la teneur en eau du sol. Pour la simulation des émissions de N_2O, les deux modèles présentèrent des performances semblables pour les quatre traitements imposés, les émissions cumulatives de N_2O étant prédites à ±15% près des valeurs mesurées. Cependant, RZWQM2 livra de meilleures estimations des émissions de CO_2 (R^2 plus élevé, erreur quadratique moyenne moins élevée) que DNDC. Les deux modèles livrèrent de bonnes estimations (en deçà de ±15% d'erreur) de l'écoulement souterrain saisonnier; cependant, les prédictions de l'écoulement souterrain journalier par RZWQM2 s'avérèrent plus précises que celles de DNDC, qui n'était pas équipé pour simuler le drainage contrôlé ou l'irrigation souterraine. Quant à la prédiction du rendement en grain du maïs et des fèves soja, les deux modèles offrirent une performance satisfaisante. Globalement, RZWQM2 s'avéra d'une plus grande applicabilité à la simulation des processus biogéochimiques des terres équipées d'un système de drainage souterrain que ne l'était DNDC.

RZWQM2 a servi à évaluer la compétence de différents MPGs envisageables à mitiger les émissions de GES provenant d'un champ de maïs équipé de drainage souterrain et opérant un système de gestion de la nappe phréatique. La plage optimale de fertilisation en azote permettant de réduire les émissions de GES tout en maintenant l'efficacité d'utilisation de l'azote et le rendement du maïs s'avéra entre 125 et 175 kg N ha^{-1}. Une application fractionnée d'engrais azoté réduisit les émissions en N_2O de 11%. Comparé au drainage libre, une irrigation souterraine sous régime de contrôle du drainage donna lieu à une augmentation des émissions en N_2O de 21%, mais une baisse de 6% des émissions en CO_2. Par rapport à une monoculture répétée de maïs, une rotation maïs-soya réduisit les émissions de GES de 20%.

Les impactes du changement climatique sur le rendement agricole, la qualité des eaux et les émissions de GES de deux champs situés dans l'est du Canada et munis de drains souterrains, furent évalués avec RZWQM2. Sous des scénarios climatiques du futur, l'écoulement moyen d'eau par les drains souterrains et la perte d'azote par ceux-ci augmenterait de 23-41% et 47-76%, respectivement. Une augmentation de la dénitrification et de la minéralisation mènerait à une augmentation de 21-25% des émissions en N_2O, tandis qu'une plus grande accumulation de biomasse de maïs, une décomposition plus rapide des résidus de culture, et une plus grande activité microbienne du sol augmenterait les émissions de CO_2 de 16%. Ces simulations ont, en outre, indiqué que le rendement du maïs diminuerait, tandis que celui des fèves soja augmenterait. De plus, le changement climatique, en augmentant les émissions de GES provenant des terres agricoles ainsi que les pertes d'azote par le chemin des eaux de drainage, aggraverait la pollution environnementale.

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Contribution of authors

This thesis has been written in manuscript-based format. Qianjing Jiang and Dr. Zhiming Qi are co-authors for all the chapters. All the modeling work, analysis of data and preparation of manuscripts were completed by the Ph.D. candidate, Qianjing Jiang, under the supervision of Dr. Zhiming Qi. Dr. Liwang Ma and Dr. Quanxiao Fang were the co-authors for the review paper in Chapter 2, part of which was published as a book chapter. The measured data in the field experiments in Chapter 3, 4 and 5 were from Dr. Chandra A. Madramootoo, and his students Dr. Ajay K. Singh, Naeem A. Abbasi and Cynthia Crézé conducted the experiment work in each chapter, accordingly. Mr. Ward Smith provided the assistance in DNDC model parameterization and paper revision and Dr. Tie-Quan Zhang was co-author for Chapter 4. Dr. Lulin Xue and Melissa Bukovsky provided future climate data for Chapter 6.

List of manuscripts based on the thesis:

Chapter 2. Jiang, Q., Qi, Z., Ma, L., Fang, Q., 2018. Modeling water quality in subsurface drained cropland using the Root Zone Water Quality Model in Bridging Among Disciplines by Synthesizing Soil and Plant Processes. In Wendroth, O., Lascano, R.J. and Ma, L. (Eds). Bridging Among Disciplines by Synthesizing Soil and Plant Processes. SA, CSSA, SSSA, Madison, WI, USA

Chapter 3. Jiang, Q., Qi, Z., Madramootoo, C.A. and Singh, A.K., 2018. Simulating hydrologic cycle and crop production in a subsurface drained and sub-irrigated field in Southern Quebec using RZWQM2. Computers and Electronics in Agriculture, 146, 31-42.

Chapter 4. Jiang, Q., Qi, Z., Madramootoo, C.A., Abbasi, N.A., Smith, W., Zhang, T.Q., 2018. Comparison of RZWQM2 and DNDC model in simulating greenhouse gas emission, crop yield and subsurface drainage. Geoderma. Submitted.

Chapter 5. Jiang, Q., Qi, Z., Madramootoo, C.A. and Crézé, C. 2019. Mitigating greenhouse gas emissions in a subsurface-drained field in Southern Quebec using RZWQM2. Science of the total environment, 646, 377-389.

Chapter 6. Jiang, Q., Qi, Z., Xue, L. and Bukovsky, M., 2018. Assessing climate change impacts on greenhouse gas emissions and crop production in tile drained field using RZWQM2. To be submitted.

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Nomenclature

The most commonly used symbols, abbreviations and acronyms are listed below. The specific symbols that are used in a particular equation or section are described at their place of appearance in the text.

C	carbon
CO_2	carbon dioxide
CD	controlled drainage
CDS (CD-SI)	controlled drainage with sub-irrigation
CH_4	methane
CREAMS	chemical, runoff, and erosion from agricultural management systems
CS	corn-soybean rotation
DNDC	DeNitrification–DeComposition
DR	tile drainage
DRP	dissolved reactive phosphorus
ET_p	potential evapotranspiration
ET_r	reference evapotranspiration
ET_{rs}	evapotranspiration
FD	free drainage
GCM	global climate model
GHG	greenhouse gas emission
GLEAMS	groundwater loading effects of agricultural management systems
IF	inorganic fertilizer
IoA	index of agreement
K_{sat}	hydraulic conductivity
LAI	leaf area index
N	nitrogen
NH_4^+	ammonium
NO_3^-	nitrate

N_2O	Nitrous oxide
NSE	Nash–Sutcliffe model efficiency
NUE	nitrogen use efficiency
Obs	observed
PEST	Parameter Estimation Software
QPSO	quantum-behaved particle swam optimization
r^2	Coefficient of determination
RCM	regional climate model
RH	relative humidity
RRMSE	relative root mean squared error
RMSE	root mean squared error
RZWQM	Root Zone Water Quality Model
SCM	solid cattle manure
SHAW	Simultaneous Heat and Water model
SI	sub-irrigation
Sim	simulated
SWC (θ)	soil water content
WFPS	water filled pore space
WTM	water table management

Chapter 1

Introduction

1.1 Background

For agricultural crops, both excess and lack of water can result in irreversible crop damages and consequently yield losses. The water table depth is affected by many factors such as precipitation, irrigation, evapotranspiration, deep seepage, runoff and the depth of drain outlet in the soil. Soil can be waterlogged when a high water table is maintained during wet period and the growth of crops will be limited because excess water results in anaerobic conditions in the root zone. Artificial drainage systems are known as an important water management to remove excess water in agricultural soil in humid and sub-humid regions. They have been widely installed in humid and cold climate regions in Eastern Canada (Morrison et al., 2014). Although subsurface drainage in agricultural fields helps to promote crop production, improve machine trafficability and reduce N_2O emissions from soil as compared to undrained fields (Madramootoo et al., 2007; Fernández et al., 2016), also leads to some environmental issues, especially increasing nutrient losses in drainage. Controlled drainage reduces N losses in drainage and increases or maintains crop yield (Madramootoo et al., 2001), since it reduces drainage outflow and enhances denitrification, thereby reducing NO_3^--N losses (Ridao et al., 1998). However, it results in more N_2O release from denitrification (Kliewer and Gilliam, 1995), due to higher soil water content under water table management.

There is a need to better understand the interactions between climate, human activities, environmental quality and food security. To assess the performances of drainage systems on crop production and water quality, field experiments have been conducted during the last few decades, while very few studies have been conducted to investigate the GHG emissions under water table management. There have been few studies of the long-term effects of agricultural management practices on GHG emissions, hydrology and crop productions, since they require long-term data collections that are laborious and costly to conduct. Nevertheless, there is a concern that climate change with increasing precipitation, rising temperature and elevating atmospheric CO_2 concentration may exacerbate the water quality and GHG emission problems, as well as reduce crop production. Especially high latitude countries, including Canada, are experiencing more changes in climate than other countries.

Agricultural systems models have been used as promising tools for simulating the interactions between climate, agricultural management, crop growth and environmental quality. Computer modeling can be a reliable approach to assess the effects of different drainage systems and management practices on the hydrological processes, crop production, and the environment (Sands et al., 2003; Morrison et al., 2014). In addition, agricultural system models enable the possibility of predicting the integrated and single weather variable effects on environment and food security under climate change. Calibrated and validated models could be applied to examine the adaptive agronomic management practices to mitigate the negative impacts of climate change.

The RZWQM2 is a powerful model in crop growth and hydrology simulation and has been extensively tested under many management practices, including tillage, cover crops, rotation, different planting dates, N and water table management. Recently, it has been modified to include the components of sub-irrigation and GHG emissions. Therefore, the focus of this study is to highlight the comprehensive interactions between weather, soil, water and crops under different agricultural management, and propose mitigation and adaption strategies based on simulations.

1.2 Objectives

The goal of this research was to quantify the interactions between agricultural management, climate change, crop growth, and environmental quality. This study employs the RZWQM2 modelling approach to assess the agronomic practices and climate change impact on crop yields, water quality, water balance, and GHG emissions. The goal was achieved through the following specific objectives:

i. To evaluate the hydrologic component of RZWQM2 (Root Zone Water Quality Model) using a comprehensive hydrological dataset including subsurface tile drainage, sub-irrigation, soil water content, sap flow and crop growth data such as leaf area index, crop yield and crop growth stages.

ii. To test RZWQM2's ability to predict GHG emissions in subsurface drained field under water table management

iii. To compare the performances of RZWQM2 and DNDC models in simulating GHG emissions, crop yield and drainage flow from a subsurface drained and corn-soybean rotated field under water table and N management.

iv. To use RZWQM2 to investigate the impacts of different agronomic management practices on long-term annual GHG emissions and propose some mitigation and adaptation suggestions based on the model simulations.

v. To use the calibrated and validated RZWQM2 to assess the climate change impacts on future GHG emissions, water cycle and crop production in Eastern Canada

1.3 Thesis outline

This thesis has been written in a “manuscript based” style. Chapter 1 is general introduction, which presents the background of the research, gaps in knowledge, and objectives of the research. Chapter 2 presents the literature review on key processes of subsurface drainage, water quality and GHG emissions in the Root Zone Water Quality Model (RZWQM2) and its applications to evaluate nitrogen and pesticide losses in tile drained fields. Chapter 3, 4, 5 and 6 present the results of model evaluations, applications, and comparisons in the forms of four research papers with connecting text. The format of the five manuscripts has been changed to be consistent with the requirements of Library and Archives Canada. Figures and tables are all presented in the end of each chapter. All the references cited in the thesis are given at the end of the thesis.

Chapter 2

Modelling environment quality in subsurface drained cropland using the Root Zone Water Quality Model (RZWQM) – A review

Qianjing Jiang, Zhiming Qi, Liwang Ma, Quanxiao Fang

Abstract

Agricultural system models are used to assess agricultural management practices and their environmental impacts. However, their application to evaluate water quality in subsurface drainage requires further investigation. Our objective was to review key processes of subsurface drainage and water quality as represented in the Root Zone Water Quality Model (RZWQM) and its application to evaluate nitrogen and pesticide losses in tile drained fields. This paper introduces the RZWQM by presenting the development and improvement of its hydrologic components, the theories used for computing the water balance, the model parameterization approaches, previous works on model evaluation and its comparison with other models, model applications to assess agricultural management and climate change impacts on hydrology, crop growth and water quality, model limitations and future work. The RZWQM is a one-dimensional biophysically-based model that has been tested and extensively used for simulating the hydrological processes and nutrient transport at the field scale under different agricultural management practices, such as tillage, cropping systems, N application, cover crops, and water table management. Future work is suggested to incorporate the fate and transport of phosphorus (P) into the model to investigate the loss of P in drainage and runoff, as well as including the water ponding module to improve its accuracy during flooding periods. Meanwhile, more evaluation is needed to further test its ability to simulate greenhouse gas emissions, N fixation, crop N uptake and soil water dynamics in frozen soils. Overall, RZWQM is a promising tool for the assessment of agricultural management strategies for scientists and policymakers.

2.1 Introduction

Subsurface drainage is been practiced widely under high rainfall and high water table conditions, including the Midwest Corn Belt of the United States, Eastern Canada, and other countries such as Portugal (Randall et al., 1997; Hat- field et al., 1998; Fisher et al., 1999; Madramootoo et al., 2007; Boulet et al., 2015). In the Midwest of the United States, drainage is necessary for the crops when the water table rises up to the root zone. It has been reported to improve the crop yield in nearly 40% of the Corn Belt states such as Illinois, Indiana, Iowa, and Ohio (Johnsen et al., 1995). In Southwestern Ontario, Canada, it is also a challenge for farmers to remove the excess water from the flat and fine textured soils during the growing seasons (Tan and Reynolds, 2003). In southern Quebec where annual precipitation is usually higher than crop water demand, drainage is important to decrease the potential of spring flooding and runoff to reduce sediments and phosphorus (P) losses to the environment (Bourke, 2011).

To optimize the soil water conditions for crops in wet regions, artificial drainage is an important water management practice to remove the excess water in agricultural soils. However, the implementation of drainage systems could result in environmental problems, especially reduced water quality. The indicators of water quality in agricultural modeling are usually described as the losses and concentration of N, P, pesticides, pathogens, and other chemicals in drainage water that affect food security and human health. To assess the performances of drainage systems on crop production and water quality, field experiments have been conducted during the last few decades to investigate the subsurface drainage impacts on crop yield (Grigg et al., 2003; Hofmann et al., 2004; Kladivko et al., 2005), nitrate, P, sulfate and pesticide losses in drainage water (Baker et al., 1975; Bengtson et al., 1990; Turtola and Paajanen, 1995), and soil erosion (Turtola and Paajanen, 1995; Øygarden et al., 1997). These field experiments indicated that subsurface drainage would improve the crop yield while increasing nutrient losses in the drainage water. However, it requires long-term data collectionthat is laborious and costly to conduct. Therefore, computer modeling is a reliable approach to assess the effect of different drainage systems and management practices on the hydrological processes, crop production, and the environment (Sands et al., 2003; Morrison et al., 2014).

Hydrologic and water quality models enable the study of different drainage systems and agricultural management practices with less time and lower cost over a long period of time for any locations with different kinds of soil types and weather conditions (Thorp et al., 2007a; Qi et al., 2011). During the last several decades, many hydrological models have been developed to simulate the process of water movement within the soil–plant–atmosphere continuum. These models are designed for different purposes, and most of them are capable of calculating the subsurface drainage, including field scale models, such as ADAPT (Alexander, 1988), CREAMS/GLEAMS (Knisel, 1980; Knisel and Turtola, 2000; Knisel and Douglas-Mankin, 2012), RZWQM (Ma et al., 2012), DRAINMOD (Skaggs, 1978), EPIC and APEX (Wang et al., 2012), and watershed models, such as BASINS/HSPF (Duda et al., 2012), SWAT (Arnold et al., 1998), MIKE-SHE (Refshaard et al., 1995), and WARMF (Herr and Chen, 2012). Although the application of these models is constrained by some limitations and needs further investigation, they have introduced the concept of systematic approaches to agricultural systems and broadened people's understanding in agricultural science (Ma et al., 2001). The DRAINMOD model has been widely used to simulate subsurface tile drainage in North America (Skaggs, 1978). It is a field-scale and process-based model that simulates the drainage flow based on water balance in the soil profile and weather information to study the multi-component drainage and water management (Skaggs et al., 2012). Subsurface drainage is calculated by a combination of the

Kirkham (1957) equation and the Hooghoudt equation (Bouwer and Van Schilfgaarde, 1963). Infiltration and runoff are calculated using the Green and Ampt Equation (Green and Ampt, 1911), and seepage is computed by Darcy's law. Evapotranspiration (ET_{rs}) is calculated from reference evapotranspiration (ET_r) according to the availability of water in soil. The CREAMS (Chemical, Runoff, and Erosion from Agricultural Management Systems) model was developed by a research team from the USDA Agricultural Research Service in 1978 to address agricultural nonpoint pollution problems (Knisel and Douglas-Mankin, 2012). It is a field-scale, one-dimensional model consisting of hydrology, erosion/sediments, and a chemical component (Knisel, 1980). The model was enhanced with hydrology and nutrient components as well as the vertical flux of pesticides (Leonard et al., 1987) and developed into GLEAMS (Groundwater Loading Effects of Agricultural Management Systems) model. The GLEAMS model was initially a water quality and soil erosion model, and was later extended with the processes of nutrient cycles, subsurface drainage flow, pesticide flow and macropore flow (Knisel and Douglas-Mankin, 2012). The ET_{rs} is estimated by Ritchie's method separately as soil water evaporation and plant transpiration (Ritchie, 1972). MACRO (macropore flow model; Jarvis, 1991) is a comprehensive model that describes the movement of water in the field and solute transport in different soil and crops. Soil water flow is simulated with Richards' equation (Richards, 1931) while the drainage flow is calculated using seepage potential theory (Youngs, 1980) and the Hooghoudt equation. A detailed description of the model is given by Jarvis (1991). These models are most frequently used for estimating soil water flow and have been successfully tested in a wide variety of soil conditions.

Root Zone Water Quality Model (RZWQM) is a one-dimensional agricultural system model that contains physical, chemical, and biological processes for simulating the movement of water, nutrients, and pesticides and growth of crops in the field under various management practices (Ahuja et al., 2000b). Agricultural management practice options are available for users, including crop cultivar selection and planting, manure application, irrigation, fertilization, pesticides and tillage. The RZWQM was designed as an integrated model that simulates the hydrology, crop growth and nutrient movement on a daily basis, with a tile drainage component from DRAINMOD. More than three hundred papers have been published to study the evaluation and application of RZWQM since it was developed.

The objective of this paper was to review RZWQM in simulating the drainage flow by discussing i) the development and improvement of the drainage module and GHG component; ii) the calibration and parameterization of RZWQM, especially for the evaluation and application of RZWQM in simulating drainage and drainage water quality; and iii) the limitations and future needs of the model. This review aims to help potential users to better understand this model and make decisions on model selections for targeted management questions regarding water quality issues, for example, the nutrient and pesticide losses in subsurface drainage and the soil profile.

2.2 The history of development of the hydrologic components in RZWQM

RZWQM was initialized by USDA–Agricultural Research Service scientists in the mid-1980s based on the need to develop a comprehensive model that could respond to various agricultural management practices (Malone et al., 2004a). Being officially released in 1992 for the first version, RZWQM is a one-dimensional model that simulates the interactions between management practices and the processes of hydrology, crop growth, nutrient transformations and pesticide transport (USDA-ARS, 1992). Since then, the model has been developed and modified to improve its applicability by incorporating the DSSAT 4.0 cropping system model for crop growth, SHAW (Simultaneous Heat and Water) for surface energy balance, and GLEAMS for water erosion. To set up the model, it requires site-specific weather inputs including precipitation, minimum and maximum daily air temperature, solar radiation, relative humidity, and wind speed. Other necessary inputs are soil nutrient and hydraulic properties, crop cultivar information and field management practices. A simple flow chart that briefly describes the model input, simulation process and model output is shown in Fig. 2.1. The soil water balance can be expressed with an equation:

$$I + P = ET_{rs} + RO + DR + LF \pm \Delta SW \qquad [2.1]$$

Where I is the irrigation amount (m), P is the precipitation amount (m), RO is the runoff amount (m), DP is the deep seepage (m), DR is the drainage amount (m), LF is the lateral flow (m) and ΔSW is the change of soil water storage (m).

To simulate the hydrologic processes, the Green–Ampt equation (Green and Ampt, 1911) is used in the model for calculating the infiltration of rain and irrigation water (Eq. [2.2]) and the Richards' equation (Eq. [2.3]) is used for calculating water redistribution in the soil profile between rainfall or irrigation events (Ahuja et al., 2000a).

The Green–Ampt equation is written as:

$$\mathrm{V} = \overline{K_s}\frac{\tau_c + H_0 + Z_{wf}}{Z_{wf}} \qquad [2.2]$$

Where V is the infiltration rate at any given time (m s^{-1}), $\overline{K_s}$ is the effective average saturated hydraulic conductivity of the wetting zone (m s^{-1}), τ_c is the capillary drive or suction head at the wetting front (m), H_0 is the depth of surface ponding (m), if any, and Z_{wf} is the depth of the wetting front (m).

The Richard's equation which was used for soil water redistribution:

$$\frac{\partial \theta}{\partial z} = \frac{\partial}{\partial z}\left[K(h,z)\frac{\partial h}{\partial z} - K(h,z)\right] - S(z,t) \qquad [2.3]$$

Where θ is the volumetric soil water content ($m^3 m^{-3}$), t is the time (s), z is the soil depth (m, assumed positive downward), h is the soil-water pressure head (m), K is the unsaturated hydraulic conductivity ($m\ s^{-1}$), a function of h and z, and S(z,t) is the sink term for root water uptake and tile drainage rates (s^{-1}).

The potential evaporation of water from the soil and crop transpiration are described by the Shuttleworth–Wallace equation (Shuttleworth and Wallace, 1985) and the soil water content matric suction relationship and unsaturated hydraulic conductivity-matric suction relationship are described by the modified Brooks-Corey relationships (Brooks and Corey, 1964). The soil water content vs. the matric suction relationship is described in Eq. [2.4] and Eq. [2.5] by Ahuja et al. (2000a):

$$\theta(\tau) = \theta_s - A_1\tau\ ; \quad when\ \tau \le \tau_b \qquad [2.4]$$

$$\theta(\tau) = \theta_r + B\tau^{-\lambda}\ ; \quad when\ \tau > \tau_b \qquad [2.5]$$

The hydraulic conductivity vs matric suction relation is expressed as:

$$K(\tau) = K_s\tau^{-N_1}\ ;\ when\ \tau \le \tau_{bK} \qquad [2.6]$$

$$K(\tau) = K_2\tau^{-N_2}\ ;\ when\ \tau > \tau_{bK} \qquad [2.7]$$

Where t is the matric suction head m, t = |h|, h is the soil water pressure head), θ_s is the saturated soil water content ($m^3 m^{-3}$), θ_r is the residual water content ($m^3 m^{-3}$), τ_b is the air-entry or bubbling suction head (m), K_s is the field-saturated hydraulic conductivity ($m\ s^{-1}$), and τ_{bK} is the air-entry or bubbling suction head for this function (m), which may equal τ_b introduced above. A_1, B, λ, N_1, N_2, and K_2 are constants.

Singh and Kanwar (1995b) modified the soil water re-distribution subroutine to simulate the fluctuations of the water table, and added a tile drainage component to RZWQM. The drainage flux is calculated using the steady state Hooghoudt equation (Bouwer and Van Schilfgaarde, 1963) as applied in DRAINMOD (Skaggs, 1978):

$$\text{DFLUX}=4.0K_e E_m\left[\frac{2.0H_d+E_m}{S^2}\right] \qquad [2.8]$$

Where S is the drain spacing (m), H_d is the equivalent depth of the impermeable layer from the center of the drain (m), DFLUX is the drainage flux (m s^{-1}), K_e is the effective lateral hydraulic conductivity (m s^{-1}), and E_m is the elevation of water table above the tile drains (m).

Johnsen et al. (1995) modified the water movement module of RZWQM to simulate the fluctuating water table and subsurface drainage by allowing the simulation of saturated flow. After the modification, the performance of RZWQM was evaluated using the field measured water table depth data for 3 years under three drainage spacings in North Carolina, and then compared with other four models including WAFLOWM, SWATRAN, DRAINMOD and PREEFLO. Calculated results of the RZWQM as well as the other models were comparable to the measured values within 20%, a result that was caused by spatial differences of hydraulic properties and model uncertainties. Xian et al. (2017) incorporated two transient methods, the integrated Hooghoudt and van Schilfgaarde equations, into RZWQM and found that the simulated drainage using transient methods was similar to that using steady state Hooghoudt equation. Meanwhile, Xian et al. (2017) also found that the simulation in hourly tile drainage peak could be improved by updating soil water re-distribution and water table depth while the rainfall was occurring, opposite to the current modeling practice of holding soil water movement and water table until the rain stopped.

Flerchinger et al. (1999) incorporated a routine for computing the snow accumulation and snowmelt into RZWQM without the soil freezing process, later the soil freezing and thawing process was incorporated into RZWQM based on the Simultaneous Heat and Water (SHAW) model by Flerchinger et al. (2000). This RZWQM–SHAW model was evaluated in a cold region in North China (Li et al., 2012), Pullman, WA and Akron, CO (Flerchinger and Cooley, 1998), indicating that the coupled model had comparable performance in simulating the soil temperature, soil water content as with the SHAW model.

Preferential flow through macropores leads to rapid movement of pesticides and other chemicals to subsurface drainage (Magesan et al., 1995; Shipitalo and Gibbs, 2000). The excess amount of precipitation and irrigation that is not infiltrated would be considered as macropore flow in the presence of macropores, or directly go to the runoff in the absence of macropores (Malone et al., 2001a). This macropore flow is an important process that has been applied to simulate pesticide transport to subsurface drainage (Chen and Wagenet, 1992; Ellerbroek, 1993; Kumar et al., 1998c; Malone et al., 2001a, 2004b). The impact of macropores on subsurface drainage has been tested under several conditions with varying success. For example, Kumar et al. (1998c) indicated no significant effect of macroporosity on annual total drainage flow by comparing the statistics when simulating drainage flow with (PBIAS ranged from -26% to 8.5%, see Table 1 for statistics) and without macropores (PBIAS ranged from -27% to -1.5%). However, the macropore option slightly improved the calculation of the timing and magnitude of drainage peaks. Jaynes and Miller (1999) suggested that the accuracy of drainage calculation could be improved with more infiltration and less runoff simulated. When the macropore option was considered, the discrepancy would be reduced by half. However, it did not improve the simulation for herbicide leaching. Abrahamson et al. (2005) conducted a sensitivity test of tile drainage to macroprosity using the data from the Cecil Piedmont region where preferential flow was observed. It was concluded that calculated drainage was similar regardless of macropore flow because the slopes were not significantly different from 1 and intercepts were not significantly different from the 0 at the 0.05 probability level. However, Malone et al. (2014a) stated that the chemical concentration in subsurface drainage flow was very sensitive to the macropore numbers.

Fox et al. (2004) modified the macropore component in RZWQM by introducing a contributing area parameter (expressed as a faction) that directly connected the macropores with subsurface drainage to improve the drainage simulation. The model was calibrated using measured hydrology data from an experimental site in Indiana, USA. For model evaluation, a tracer and a pesticide were simulated; however, it was found that RZWQM failed to predict the peak concentrations of the tracer and pesticide, which was caused by the chemical buildup at the top of the water table, because RZWQM did not simulate chemical movement inside the water table. Therefore, the RZWQM was modified by incorporating an express faction into the macropore component, which allowed the macropore flow to enter into the drainage directly when the water table reached above the drain depth. Simulated results after model modification indicated that the modified RZWQM estimated the pesticide concentration in drainage with a PBIAS of 21%, while the previous version underestimated the value by 93%, because the modified version was able to capture the earlier peaks in tracer and pesticide concentration. The model results could be improved with chemicals being transported below the water table by diffusion or turbulent flow, rather than using an empirical express factor. To study the bacteria transport in the soil profile, subsurface drainage and runoff, Guzman and Fox (2011) modified RZWQM by incorporating bacteria transport and biopore routines into the model. The statistics of model evaluation results (PBIAS and RRMSE) showed an improvement of the modified RZWQM in calculating the increased drainage flow and bacteria transport in response to irrigation and rainfall events, as well as capturing the timing and magnitude of drainage flow peaks and trend of bacteria concentration.

An ongoing effort has been made to develop a stand-alone subroutine in RZWQM to simulate the fate and transport of P in subsurface drained field (Sadhukhan et al., 2017). The developed P module is designated in simulating both dissolved reactive P (DRP) and particulate P (PP) losses through surface runoff and tile drainage while special attention has been paid to simulate P loss through tile drainage using most recently updated sciences in the fate and transport of P in agricultural systems. The developed P subroutine was tested against field measured DRP and PP in tile drainage and surface runoff at a drainage site in 2008 to 2012 near Harrow, ON, Canada. The preliminary results suggest that this new P module is capable of simulating P losses with NSE > 0.5, PBIAS within ± 0.25 and IoA > 0.75 (see Table 1 for statistics) in both calibration and validation periods. This stand-alone module needs to be coded in the main stream of the model and tested with more field measured data; a user-friendly interface should be developed for a better application of this module.

Not all the improvements on RZWQM were included in the currently released version of RZWQM (version 4.0). An early improvement to use soil water dependent macropore size by Hua (1995) was never incorporated in the RZWQM, neither the bacteria (Guzman and Fox, 2011) and rainfall interception by crop canopy (Kozak et al., 2007). Effort is underway to assemble all the new improvements into an updated version after extensive testing.

2.3 The nutrient component in RZWQM2

2.3.1 The nitrification, denitrification and organic matter decay processes in RZWQM2

The OMNI program, developed as a submodel of RZWQM2, simulates the organic matter and nitrogen cycling pathways, including mineralization and immobilization, inter pool transfer of C and N, aerobic nitrification, anaerobic decay and denitrification, microbial biomass growth and death, etc. In OMNI, the decayed soil organic carbon (SOC) is channeled in three directions: transfer to other organic matter pools, assimilation into biomass, or as a CO_2 sink *via* biomass respiration. Drawing on a fraction of the biomass pool lost to inter-pool transfer, OMNI converts the remaining decayed organic matter to biomass carbon by way of an efficiency factor, and considers the remaining organic carbon as being the result of CO_2 from aerobic respiration going to a C sink (Ahuja et al., 2000b). The organic matter is divided into five pools: (i) plant or other organic structural material (slow pool), (ii) plant or other organic metabolic material (fast pool), including crop residues, manure, and other organic materials, (iii, iv, v) fast, medium and slow decaying SOM pools (Fig 2.2 and 2.3). Microbial biomass aerobic and anaerobic respiration result in C source storage from CO_2 and CH_4, respectively. Then the CO_2 and CH_4 are used as C resource for nitrification and aerobic organic matter decay, respectively (Ahuja et al., 2000).

In RZWQM2, nitrification rate (R_{nit}) is computed using either zero-order or first-order kinetics, depending on the NH_4^+ concentration, and denitrification rate (R_{den}) is calculated using first order kinetics (Ahuja et al., 2000; Fang et al., 2015):

$$K_{nit} = F_{aer} \times (\frac{k_b T}{h_p}) \times A_{nit} \times \exp(-\frac{E_{nit}}{R_g T}) \times \frac{[O_2]^{0.5}}{[H^{kh} {\gamma_1}^{kh}]} \times P_{aut} \quad [2.9]$$

$$R_{nit} = -K_{nit} \times s_{12} \times \gamma_1 \quad [2.10]$$

$$K_{den} = F_{anaer} \times (\frac{k_b T}{h_p}) \times A_{den} \times \exp(-\frac{E_{den}}{R_g T}) \times \frac{[C_s]}{[H^{kh} {\gamma_1}^{kh}]} \times P_{ana} \quad [2.11]$$

$$R_{den} = -K_{den} \times s_{11} \times \gamma_1 \tag{2.12}$$

Where K_{nit} and K_{den} are rate coefficients for nitrification and denitrification, F_{aer} and F_{anaer} are soil water factors; k_b is the Boltzman constant (1.383×10^{-23} J K^{-1}); T is soil temperature; h_p is the Planck constant (6.63×10^{-34} J s); R_g is the universal gas constant (1.99×10^{-3} kcal mol^{-1} K^{-1}); E_{nit} and E_{den} are the apparent activation energy for nitrification and denitrification processes (kca $mole^{-1}$), respectively; A_{nit} and A_{den} are nitrification and denitrification rate coefficients (s day^{-1} $organism^{-1}$), respectively; $[O_2]$ is oxygen concentration in soil water (moles O_2 per liter pore water); H is hydrogen ion concentration (moles H per liter pore water); kh is hydrogen ion exponent for decay of organic matter microbes, nitrification and denitrification (=0.167 for pH ≤ 7.0, and = -0.333 for pH >7.0); γ_1 is the activity coefficient for monovalent; C_s is weighted carbon in the soil (μg C g $soil^{-1}$); P_{aut} is the autotrophic biomass population of nitrifiers (organisms g $soil^{-1}$); P_{ana} is population of anaerobic microbes (organisms g $soil^{-1}$); s_{12} is the concentration of NH_4^+ (moles NH_4^+ per liter pore water per day); s_{11} is the concentration of NO_3^- (moles NO_3^- per liter pore water per day).

In RZWQM2, the organic matter is divided into five pools: plant or other organic structural material (slow pool), plant or other organic metabolic material (fast pool), and fast, medium, and slow decaying soil organic matter. The basic equations of computing the organic matter decay rates for all the pools are the same, except the user-supplied rate coefficients. The decayed soil organic carbon flows in three directions: transferred to other organic matter pools; assimilated in biomass or loss as CO_2 via biomass respiration (Ahuja et al., 2000). It should be noted that the CO_2 emission from root respiration and assimilation by plants from photosynthesis were not considered in this model.

The equations for computing aerobic decay of organic matter are also first-order, and the coefficient for decay ($r_{dec,i}$) is (Ahuja et al., 2000):

$$K_{dec,i} = F_{aer} \times (\frac{k_b T}{h_p}) \times A_i \times \exp(-\frac{E_a}{R_g T}) \times \frac{[O_2]}{\left[H^{kh} {\lambda_1}^{kh}\right]} \times POP_{het'} \quad [2.13]$$

$$r_{dec,i} = K_{dec,i} \times S_i \quad [2.14]$$

Where i is the organic matter pool index, $1 \le i \le 5$, $K_{dec,i}$ is the rate coefficient for decay, $POP_{het'}$ is the population of aerobic heterotrophic microbes (organisms gm soil^{-1}), E_a is the apparent activation energy for decay (kca mole^{-1}), S_i is the carbon substrate concentration (μg C gm soil^{-1}).

2.3.2. The development of RZWQM2 for simulating N_2O emissions from nitrification and denitrification

Fang et al. (2015) improved RZWQM2 by incorporating the algorithm for computing N_2O emission from nitrification based on the NOE model and N_2O emission from the denitrification algorithm in the DAYCENT model to predict N_2O emission from the soil profile.

The algorithm for computing N_2O emission from nitrification was implemented from NOE model by Fang et al. (2015) as followed:

$$N_2O_{Nitri} = Fr_{N_2O\_Nit\_NOE} \times SW_{N_2O\_Nit\_NOE} \times R_{nit} \quad [2.15]$$

$$SW_{N_2O\_Nit\_NOE} = \frac{0.4 \times WFPS - 1.04}{WFPS - 1.04} \quad [2.16]$$

The algorithm for computing the N_2O emission from denitrification was taken from the DAYCENT model:

$$N_2O_{Den} = Fr_{N_2O\_Den\_DAYCENT} \times R_{Den} \quad [2.17]$$

$$Fr_{N_2O\_Den\_DAYCENT} = \frac{1}{1+R_{NO\_N_2O}+R_{N_2\_N_2O}} \quad [2.18]$$

where $Fr_{N_2O\_Nit\_NOE}$ and $Fr_{N_2O\_Den\_DAYCENT}$ are the fractions of nitrification and denitrification for N_2O emissions, $SW_{N_2O\_Nit\_NOE}$ is the soil water factor for the oxygen availability effect on N_2O emission during nitrification, $R_{NO\_N_2O}$ is the ratio of NO to N_2O and $R_{N_2\_N_2O}$ is the ratio of N_2 to N_2O.

2.4 Model Parameterization for Subsurface Drainage Simulations

2.4.1 Model calibration

Model calibration is the process to minimize the differences between calculated and measured values by adjusting model parameters, usually through the trial and error procedure. The RZWQM input parameters could be obtained from field measurements; however, most of these parameters are not easy to measure, thus the model calibration procedure usually requires parameters estimated from literature or experience (Malone et al., 2001b). To calibrate the subsurface drainage component of hydrologic models like RZWQM and DRAINMOD, an accurate estimation of ET_{rs} is crucial since very small changes in ET_{rs} prediction would lead to significant changes in drainage (Thorp et al., 2009). A protocol for parameterization and calibration of RZWQM in field research was proposed by Ma et al. (2011). It was suggested that water table depth should be evaluated for a reasonable hydrology simulation by verifying the leakage rate, lateral hydraulic gradient, ET, runoff, deep seepage and lateral flow. The field capacity and slope of soil water retention curve were crucial parameters that affect the water movement and thus drainage amount. In addition, the lateral K_{sat} should be calibrated for each soil layer for calculating the drainage flow. The detailed information in choosing hydraulic parameters and variables for calibrating the hydrologic components are listed in Table 2 and some examples related to drainage and drainage water quality calibration in RZWQM are shown in Table 3.

Trial-and-error is the most traditional and widely used process for RZWQM calibration. However, it is subjective in a way that two users may end up with two different sets of parameters, while the automatic calibration is relatively objective and efficient (Ma et al., 2012). In addition, two sets of totally different parameters would lead to similar calculated results (Ma et al., 2012). This subjectivity would greatly affect the manual calibration process (Xi et al., 2016). Therefore, several automated calibration tools and methods have been developed for RZWQM parameterization.

The PEST (Parameter Estimation Software) was developed for model parameterization for underground water models (Doherty and Hunt, 2010). Parameters in groups can be obtained automatically from this software when their ranges are set by the users. It was incorporated into RZWQM to enhance efficiency of model calibration and to help in parameter selection for users' convenience by allowing sensitivity and uncertainty analysis (Ma et al., 2012). Nevertheless, as an automated calibration method, PEST offers more objective, systematic and repeatable parametrization when compared with the trial-and-error calibration process (Malone et al., 2014a). Examples of using PEST for RZWQM parameterization have been introduced by Malone et al. (2010), Fang et al. (2010), Nolan et al. (2011), and Anar and Lin (2016). Despite its capability of optimizing parameters for simulation results and emphasizing model outputs defined by users, it requires appropriate initial values and a cautious decision making in selecting the weighting factors in the objective function (Xi et al., 2016). In addition, it has the limitation that the fixed objective function format in PEST software could not be freely modified when necessary (Xi et al., 2015).

Therefore, new approaches are required for RZWQM calibration are required for optimizing the simulation results. Xi et al. (2015) calibrated the RZWQM automatically using a quantum-behaved particle swarm optimization (QPSO) algorithm for a subsurface drained field in Iowa as previously calibrated by Qi et al. (2011). The QPSO algorithm, introduced by Sun et al. (2004), is an uncertainty searching technique to find optimal solutions. The calibration results provided by the QPSO method were satisfactory compared with the traditional manual calibration method (PBIAS, NSE and RSR within the acceptable range), which indicated its promising applicability in automatic parameterization of RZWQM. However, this method requires large computation and intensive model runs, especially for comprehensive agricultural models like RZWQM which might take several minutes to run a single scenario, and the whole parameterization process could require running thousands of times and take weeks to finish the computation. Thus Xi et al. (2016) developed a surrogate based optimization algorithm to calibrate the RZWQM that aimed to improve the efficiency and reduce the computational cost for global parameter optimization. Calibration results suggested that this method performed well in parameterization for RZWQM with less computational time and cost.

2.4.2 Sensitivity Analyses

Sensitivity analyses help to determine the most important parameters for certain outputs and the sources of errors during a simulation (Ma et al., 2000). According to the Hooghoudt's steady state equation which is used to calculate the subsurface drainage in RZWQM, the drainage spacing and depth are important input for computing subsurface drainage (Ahuja et al., 2000a). A sensitivity analysis before model calibration for Southern Ontario, Canada, indicated that the tile drainage flow was most sensitive to h_b, K_{sat}, lateral K_{sat}, moderately sensitive to drainable porosity, and less sensitive to tile drain depth (Ahmed et al., 2007a). Ma et al. (2007a) tested the sensitivity of tile drainage flow to soil hydraulic parameters in RZWQM using Latin Hypercube Sampling. To achieve this goal, soil hydraulic parameters were measured from the experimental site and simulation results were compared between scenarios with measured and default parameters. Simulated soil hydrology was found to be better with the measured soil parameters than the default parameters suggested by the soil texture class within RZWQM. Sensitivity analysis indicated that the subsurface drainage flow was most sensitive to the hydraulic gradient, sensitive to saturated soil water content and lateral K_{sat} while not sensitive to bubbling pressure and K_{sat}. Ma et al. (2000) also stated that the hydrologic outputs of RZWQM were more sensitive to the average K_{sat} for all soil layers than K_{sat} of the individual soil layers. Sun et al. (2016) applied the GLUE (generalized likelihood uncertainty estimation) method to assess the uncertainty and sensitivity of RZWQM. To start the uncertainty analysis, model calibration was conducted first against two years of measured data from an experimental site in Beijing using the PEST method. Then 25 parameters most related to soil water content, NO_3–N in soil profile, maize grain yield and wheat grain yield were suggested by PEST were consequently selected for sensitivity analysis. The sensitivity test listed the parameters that affected the four outputs mentioned above and provided an example for model parameterization.

2.5 Model Evaluation and Applications

The drainage component of RZWQM has been extensively evaluated in North America. The first evaluation for the drainage component of RZWQM was made in Iowa, USA, by Singh and Kanwar (1995a). The model was calibrated using the measured subsurface drainage flow data under four different tillage treatments in 1990 and validated using the same data from 1991 to 1992 that were collected from the NERC water quality research site at Nashua, Iowa. The statistics of both calibration and validation were within the acceptable range, with r^2 varying from 0.49 to 0.69 and PBIAS within 13%. The model was proved to be capable of simulating the time of drainage peaks very close to the recorded time, and the calculated drainage flow under different tillage practices indicated similar trends as measured. Meanwhile, Singh and Kanwar (1995b) extended the previous modified RZWQM model for simulating the N losses in subsurface drainage water. The further modified model was later evaluated to study the impact of different tillage practices on N concentration and N losses in drainage water by comparing simulated results with measured data collected from 1990 to 1992 in Nashua, IA. The model evaluation indicated the modified RZWQM was capable of estimating N concentrations under different tillage systems during the simulated years. However, the RZWQM failed in calculating tillage effects on N losses in drainage in 1991 and 1992.

In most cases, the RZWQM was judged as satisfactory in calculating the drainage flow and chemicals in drainage flow. Bakhsh et al. (2004a) evaluated the model with the measured data from a field in the Walnut Creek watershed, IA, showing that the measured drainage was comparable to the measured data with the NSE of 0.99, and the NO_3–N losses in drainage water was calculated with the NSE value of 0.80. In the coastal area of Canada in Nova Scotia, the performance of RZWQM was evaluated for simulating the subsurface drainage flow in a shallow drained soil (Akhand et al., 2003). Calculated drainage amount agreed with the measured values with r^2 of 0.60 and 0.57, respectively, for calibration and validation, indicating the wide adaptability of RZWQM for subsurface drainage simulation under various climate and soil conditions.

The performance of RZWQM on simulating the subsurface drainage and chemical transport under various management practices, weather and soil conditions has been widely evaluated, but few studies have been conducted to test its ability in calculating the pesticide transport, macropore flow, and surface runoff in tile drained field. Kumar et al. (1998a) calibrated the RZWQM (version 3.25) using the measured daily drainage and atrazine concentration data from Nashua, IA under two tillage systems in 1990 and validated it using data from 1991 to 1992. The PBIAS indicated that simulated drainage flow, and atrazine loss to tile drains matched closely with the measured values for the three years under two tillage systems, and the simulated timing of atrazine concentration were comparable with the observation. Later, Malone et al. (2014a) evaluated the model's ability in calculating the pesticide transport using the data from a six-year field study (1990 to 1995) from the same location in Iowa. Results of both evaluations suggested that RZWQM was able to simulate the process of pesticide transport in subsurface drainage flow under two tillage systems for continuous years. Using hourly tile drainage data from Ontario, Canada, and Iowa, United States, Xian (2017) found that the hourly peak of tile drainage could be improved by adding the macropore component of RZWQM. However, the macroporosity and pore radius parameters in the model were proved to be insensitive. Lu (2015) first tested RZWQM in simulating surface runoff in a subsurface drained field in Ontario and found that the model well simulated surface runoff in a field with free drainage conditions but for the controlled drainage with sub-irrigation field the simulation was not satisfactory.

Since the RZWQM provides options for many different agronomic management practices including manure application, irrigation, fertilization, pesticides, tillage, subsurface drainage, controlled drainage and irrigation, it has been widely used in simulating the impact of agricultural management practices on hydrology, water quality, and crop production. The performance of RZWQM in calculating subsurface drainage flow and water quality has been extensively reported under different conditions, such as manure applications in Iowa (Kumar et al., 1998b), tillage systems (Kumar et al., 1998a; Ma et al., 2007b; Malone et al., 2014a), pesticide application rates (Malone et al., 2014a), N application management (Azevedo et al., 1997; Bakhsh et al., 2001; Qi et al., 2012), and winter cover crops (Abrahamson et al., 2006; Qi et al., 2011). Numerous model validations and evaluations were completed to show the applicability of RZWQM in simulating the management practices effects (Hanson et al., 1998).

2.6 Water Table Management

Water table management, including the subsurface drainage, controlled drainage and subsurface irrigation systems, has been reported as an effective approach to improve the water quality by reducing the N losses in drainage water (Elmi et al., 2000; Madramootoo et al., 2001; Drury et al., 2014). RZWQM has been applied as a tool to develop suitable water table management practices under certain weather and soil conditions. Studies on the application of RZWQM in this context informed how different water table management strategies affect the water balance and N cycling across the Midwestern United States (Thorp et al., 2007a, 2008). The long-term simulation results from 48 locations across the Midwestern U.S. indicated that water table management demonstrated a significant impact on the subsurface drainage amount. Controlled drainage resulted in, on average, a reduction of drainage flow by 53% for 25 yr for all the locations. The reduction of drainage flow differed among the locations, which varied from 35% to 68% accordingly when moving from northwest to the southeast across the region. The results also provided a reference for the water table management impact on reducing N loss in drainage across different locations in the United States. According to another simulation over 23 yr to study the agricultural management practice impacts in Nashua, IA, by Ma et al. (2007b), the subsurface drainage water was on average 30% lower in the controlled drainage system than the free drainage system. Consequently, the N loss in drainage water was also reduced by 29% when controlled drainage was applied. Based on a long-term RZWQM simulation (1996–2008), Fang et al. (2012) studied the effects of controlled drainage on N loss to subsurface drainage and also found that N loss could be reduced by 39% (9.3 kg N ha^{-1}) after switching from free drainage to controlled drainage at N fertilizer application rate of 140 kg N ha^{-1}. The averaged measured and simulated monthly tile flow, flow-weighted nitrate N concentration, and nitrate N losses were plotted in Fig. 2.4.

These model results were in agreement with some reported field experiments. For example, Helmers et al. (2012) reported that annual NO_3–N loss from 2007 to 2010 was reduced by 36% for controlled drainage at a site with silty clay loam soil in Iowa. The reduction of N and P loss by controlled drainage compared with a free drainage system varied from 30% to 50% depending on soil type, climate, drainage system design and management based on some field studies in the United States (Evans et al., 1995). In southwestern Ontario 14% and 26% reductions of N loss from controlled drainage was reported under tilled and no-till systems, respectively (Tan et al., 1998). A two-year field study that was conducted on a loamy sand in Sweden from 1998 to 1999 compared the nitrate loss of controlled drainage with free drainage and resulted in the total amounts of nitrate in drainage of 78% and 94% less, while the P loss were 58% and 85% less in 1998 and 1999, respectively (Wesström et al., 2001).

2.7 Fertilizer and Manure Management

Although subsurface drainage has been proven to be an effective management practice to improve the growth conditions for crops, its side-effects on water quality is also of great concern to the environment. Since RZWQM was designed with many options for applying different sources of N, and for varying the application timing and rate, it has been tested in simulating different N management practices impact on N losses in drainage water.

Azevedo et al. (1997) indicated an increase of N losses in drainage and higher crop yield with increasing N application rates, but the increment of N losses and crop production were not linearly proportional to the extra N application rates. In addition, they showed no significant difference in N loss and crop yield between one-time N application and several split applications when the total amount was unchanged in this research. Kumar et al. (1998b) evaluated the RZWQM in simulating the drainage flow and water quality under manure applications in Iowa. The PBIAS of simulated annual drainage flow was in the acceptable range compared to the measured values for the three plots in both years (within 3.1% and -10.9% for calibration year and validation year, respectively), and daily drainage as well as the trend matched with the measured values except a few underestimations of drainage peaks in early spring due to snow melt. Meanwhile errors in estimating ET_{rs} in September and missing values of some break point rainfall data might also result in inaccuracy of drainage calculation. Generally, the model was capable of calculating annual drainage flow, its timing and N loss in drainage water. However, the development of snow accumulation, freezing and thawing process components was suggested for model improvement. Moreover, the macropore flow component, as well as the estimation of ETrs should also be improved to enhance model performances.

Qi et al. (2012) reported a long-term simulation using RZWQM to investigate the effect of different N application rates on N loss in a subsurface drainage system in north-central Iowa (Fig. 2.5). Crop yield was found to be reduced with decreasing N application rates. Meanwhile, the authors suggested an N appli cation rate to meet the requirement of the water quality standard (maximum contaminant level) in the Iowa region, which was similar to the recommended rate from the field study. Malone et al. (2007) applied the RZWQM to quantify the long-term effects on crop production and water quality in subsurface drainage water with different N varieties, timing and rates of chemical fertilizer and swine manure. The overall calculation indicated increasing corn yield and N losses in response to higher N applications. Simulations of long term N application impacts on drainage water quality and crop production have been conducted in Ontario, Canada. Ahmed et al. (2007b) indicated the side-dressing of N application would lead to a slight reduction of N losses in drainage and significant corn yield reduction on the silt loam soil, while it resulted in great reduction of both N losses in drainage and corn yield on sandy loam soil. McKague et al. (2006) tested several N management practices that include MERN (the Most Economic Rate of Nitrogen), side-dress N application, pre-plant N application, split N applications, preside-dress N test (PSNT), and reduced N application through crop rotation. They suggested the N application timing and rate were important to reduce the N losses to drainage water. For example, it was found that split N applications could reduce N loss to drainage by 7.6% compared with MERN. This research provided a good example of using agricultural models to develop the best management practices for optimizing crop production and mitigating its side effects on water quality as well.

Bakhsh et al. (2001) found that RZWQM overestimated the N losses in drainage during the soybean years that required improvement for N_2 fixation and N uptake process. Similar suggestions for improving the RZWQM with regard to simulating N fixation of soybean, and plant N uptake were proposed by Ma etal. (2007b) when investigating the effects of crop rotation, tillage, and controlled drainage on N losses in drain flow. The calculated tile flow, N losses in drainage water during the corn years, and yields of both corn and soybean matched well with the measured values. Subsequently, six different N application rates from zero to a plateau value were simulated using the RZWQM to investigate the N application impact on corn yield and water quality. It was concluded that RZWQM has the potential to assess the N application effects on water quality and corn yield.

2.8 Crop Rotation, Cover Crops, Tillage, and Crop Residue Removal

The impacts of other agronomic management practices including crop rotations, winter cover crops, tillage, and crop residue removal on water resources and crop production have been investigated using RZWQM. According to a long-term simulation in Southern Ontario, Canada, by Ahmed et al. (2007b), RZWQM calculated greater reduction of N losses in drainage on a silt loam soil than on a sandy loam soil when changing the rotation from corn-soybean to corn-soybean-soybean. As stated in the model evaluation part, the RZWQM has been evaluated in Nashua, IA, United States, with 26 yr of data (1978–2003) and its performance was satisfactory in simulating the hydrology components of water table, soil water storage and tile drainage flow, as well as the N balance, crop yield and biomass using the statistics of r^2 and RMSE (Ma et al., 2007c). Figure 2.6 shows the responses of RZWQM to 26 yr of weather pattern in terms of the crop yield, tile flow, N loading in tile flow, and flow-weighted N concentration in tile flow across all treatments. Statistics listed in Fig. 2.6 indicated good performance of RZWQM in simulating the trend of yield, annual tile flow, and N loading in tile flow, despite some inaccuracies because of the presence of flooding in the years of 1993 and 1999. Overestimation of corn yield in some years resulted from waterlogging, which RZWQM did not consider. After the model evaluation, the long-term management impacts on hydrology and crops was simulated (Ma et al., 2007b), in which results showed 14% less drainage under the corn–soybean rotation than under continuous corn planting, which can be explained by the difference of ET_{rs} between corn and soybean. Yearly drainage was similar during the years when ET_{rs} was similar for the two crops.

Malone et al. (2007) simulated the long-term effect of winter cover crops on N loss and concluded that N loss can be reduced under winter cover crop without decreasing the corn yield. Qi et al. (2011) investigated the long-term impact of winter rye cover on water cycling and N dynamics under a soybean-corn rotation system. Before the long-term simulation, the model was calibrated and validated against the daily drainage flow under four different treatments (winter rye growth prior to corn in odd years and prior to soybean in even years (TRT1), winter rye cover crop growth prior to soybean in odd years and prior to corn in even years (TRT2), corn in odd years and soybean in even years without cover crop (CTRL1), and soybean in odd years and corn in even years without cover crop (CTRL2). The measured and simulated daily drainage for 2007 and 2008 were compared to evaluate the performance of RZWQM with regard to simulating daily drainage (Fig. 2.7). As the model calculation of drainage as well as other components have been judged as "satisfactory" after statistical analysis, results of long-term simulation indicated that winter rye cover crop reduced annual subsurface drainage and NO_3–N loss by 11% (29 mm) and 22% (11.8 kg N ha-1), respectively, and increased annual ET by 5% (29 mm) through a long-term (40 yr) simulation using RZWQM. Singer et al. (2011) found that winter cover crop helped to reduce the annual N loss from tile drainage by 24% and 19% in the corn-soybean and the corn-corn–soybean rotation, respectively. The reduction of N loss benefited from cover crops has been reported by Kladivko et al. (2014), who simulated the corn–soybean rotation and continuous corn planting in the states of Ohio, Indiana, Illinois, Iowa, and Minnesota in the Mississippi River Basin using RZWQM. The authors demonstrated 20% less N loss to the Mississippi River under winter rye cover crop in the Midwestern United States, which indicated the cover crop strategy as an effective adoption for reducing N losses and improving water quality in this area. Gillette et al. (2017a) simulated the NO_3^- losses in subsurface drainage in central Iowa over 9 yr from 2002 to 2010 and found average measured and RZWQM simulated drain flow N concentration with winter rye cover crop were 60% and 54% less than without cover crop.

Ma et al. (2007b) reported the impact of four different tillage practices on hydrology, including no-till (NT), ridge till (RT), chisel plow (CP) and moldboard plow (MP). Since different tillage practices only resulted in changes in soil hydraulics and mixture of crop residue in soil surface for a very short period after the application in the model, the results showed the drainage flow under NT was 7% to 14% higher than MP and 2% to 5% higher than CP. It was indicated that the tillage effects on drainage were closely dependent on the other management and weather conditions, and their effect on N loss in tile flow was the least compared to other management practices. A recent study by Shipitalo et al. (2016) reported a simulation on the effect of the removal of corn stover on pesticide loss through drainage water. It was indicated that residue removal would result in decreasing subsurface drainage because of the reduction of crust conductivity and soil macroporosity. Moreover, an increase in pesticide losses in drainage was found to be due to pesticide sorption reduction, which was caused by more water moving through fewer macropores.

2.9 Climate Change Issues and N_2O emissions

Due to its capability of simulating hydrological processes, crop production, and nutrient dynamics corresponding to different agricultural management practices, as well as the reasonable response to the elevated CO_2, RZWQM could serve as a tool to assess the climate change impacts on future hydrologic cycle and crop production, as well as to investigate adaptation and mitigation methods toward the predicted situations. Ko et al. (2012) simulated the future climate change impacts on crop production in the Central Great Plains of the United States using RZWQM model. Future weather data were generated as the input for RZWQM to investigate ambient temperature, CO_2 and precipitation effects on crop yields. Recently, a RZWQM simulation by Wang et al. (2015) reported that under future climate (2045–2064), subsurface tile drainage, NO_3–N loss and flow-weighted average NO_3–N concentration would increase by 15%, 34% and 16%, respectively in Iowa, USA. The grain yields of soybean and corn in the future under different scenarios are shown in Fig. 2.8. Simulated soybean yield would be increased by 28%, which mainly resulted from the enhancement of CO_2 concentration and photosynthesis rate while the increased temperature has negligible impact. Simulated corn yield would decrease because of shorter growing days and earlier maturity dates due to increased air temperature. Although the wind speed, relative humidity and solar radiation have great impact on the simulated ET_{rs} thus affect the crop yield and water balance, the predicted future changes in these three weather variables were very minor thus they had negligible impact on crop production and water balance.

Gillette et al. (2017) tested the modified RZWQM2 model in predicting the effect of tillage and N fertilization amount on N_2O emissions in an irrigated corn field in Colorado, indicating that it slightly under estimated N_2O emissions by 1.5% and 7.1% under no-tillage and conventional tillage, respectively. Jiang et al. (2017) evaluated RZWQM2 for predicting N_2O and CO_2 emission in a subsurface drained field in Southern Quebec under water table management, and used the calibrated model to investigate different agronomic management impacts on GHG emission. With the available simulated results for long term climate change impacts on N losses in water, N_2O emission and crop production, the modified RZWQM was applied by Wang et al. (2016) to test different management practices in mitigating the negative effects. In this research, various management practices were investigated under future climate data which included different N application rates, tillage systems, new crop cultivars, water table management practices, and planting date. Long term simulation results suggested that (i) increasing N application led to higher corn yield and more N losses in drainage; (ii) the tillage systems showed no obvious influence on corn yield and N loss in drainage; (iii) new corn cultivars were proposed for increasing yield and reducing N_2O emissions, N losses in drainage in the future; (iv) the controlled drainage reduced the drainage flow and N losses in drainage by 6% and 13%, respectively, while it had very limited impact on corn yield; and (v) delaying planting date could be an effective way to promote crop yield.

2.10 The Comparisons of RZWQM with other Models

The performance of RZWQM for simulating the hydrological components has been compared with some other similar models, indicating that RZWQM performed equivalently to, or even outperformed similar models. Singh et al. (1998) compared the performance of both RZWQM and DRAINMOD in simulating the climate and management practices impacts on tile drainage water quality. Simulated results showed that both models adequately simulated the effects of different management practices and rainfall amount on N losses in drainage water, but better calculation of N losses was found in DRAINMOD than in RZWQM, which was because DRAINMOD had the algorithm to simulate NO_3–N transformation under controlled drainage at that time while RZWQM did not. Another comparison between DRAINMOD and RZWQM in simulating the hydrology and N dynamics of a field in Iowa was reported by Thorp et al. (2009). After the calibration and validation of both models using the same dataset, the statistics of relative root mean squared error (RRMSE) and Nash–Sutcliffe model efficiency (NSE) indicated that both models performed well in simulating the yearly drainage and daily drainage for the continuous 10 yr. However, with a greater control over the crop component by users, DRAINMOD simulated the NO_3^- losses in drainage more accurately than RZWQM, while RZWQM simulated much more details of the processes with less required inputs. A comparison between RZWQM and GLEAMS was made by Chinkuyu et al. (2004) in simulating the processes by calibrating the two models using the field experimental data from the fields at the USDA research center in Beltsville, MD. Simulated results from both models suggested the presence of a seepage zone that helped to improve the accuracy in calculating the soil water content and surface runoff. However, statistical results of PBIAS, root mean squared error (RMSE), coefficient of determination (r^2), NSE and index of agreement (IoA) all indicated a better capability of RZWQM than GLEAMS in calculating the effects of the seepage zone on soil water content and surface runoff, which was explained by RZWQM using the Green-Ampt infiltration method while GLEAMS using NRCS (Natural Resources Conservation Services) curve number method. Another comparison reported by Ma et al. (1999) suggested that RZWQM calculated the partitioning of ET to soil water evaporation more reasonably while GLEAMS tended to overestimate it. The performance of the MACRO model in simulating water discharge under a subsurface drainage system from an experimental site in Western France has been compared with the RZWQM by Kuzmanovski et al. (2015). The comparison between these two models indicated a better simulation by RZWQM rather than MACRO in simulating the overall drainage flow in terms of RMSE, and the RZWQM model simulated the timing of peak flows while MACRO model missed most of the major peaks for drainage events.

2.11 Summary and Conclusion

The RZWQM is a physically-based agricultural system model that integrates the physical, chemical, and biological processes for simulating the movement of water, nutrients, and pesticides and growth of crops in the field under various management practices. The drainage component was developed and modified to meet certain research goals, extending its availability for simulating the hydrology and drainage water quality under different conditions. Experienced users can calibrate the model manually by a trial-and-error method, but other automatic calibration methods are also available such as PEST, quantum-behaved particle swarm optimization (QPSO) algorithm and surrogate-based optimization algorithm. The model has been evaluated as satisfactory and applied successfully in many regions for simulating the impact of agricultural management practices and climate change on hydrology and water quality. The RZWQM provides an efficient way to qualify and quantify the agronomic management effects on water balance, quality and crop production, therefore gives solutions to optimize crop growth conditions and improve water quality, and provides directions for future field experiments. Overall, it is a very comprehensive biophysically-based model and its performances in simulating the hydrologic process, crop growth as well as the C/N cycle are comparable to many hydrological models. The RZWQM integrates the modules from various models, which makes the model applicable to many agricultural systems and environmental issues. However, it also brings a formidable task for new users to calibrate this model. In addition, many other limitations still exist in the model. For example, since it is a one-dimensional model, it does not simulate a regional water table that may affect tile flow. Meanwhile the biological, chemical and physical processes within the soil profile are much more complex and may be influenced by many uncontrollable factors. Moreover, the quality of measured data from field experiments has crucial impact on the model performance. Furthermore, the model does not consider the water ponding and flooding that may also affect its accuracy in simulating the soil water dynamics and crop growth. Finally, because P is one of the major factors of nonpoint source pollutions that contribute to eutrophication, the ongoing effort in developing P subroutine for RZWQM should be encouraged and continued. Therefore, future work is suggested to complete the P cycle component and water ponding for the model, and more evaluations are required to further test its ability in simulating greenhouse gas emissions, N fixation, crop N uptake and water balance in frozen soil.

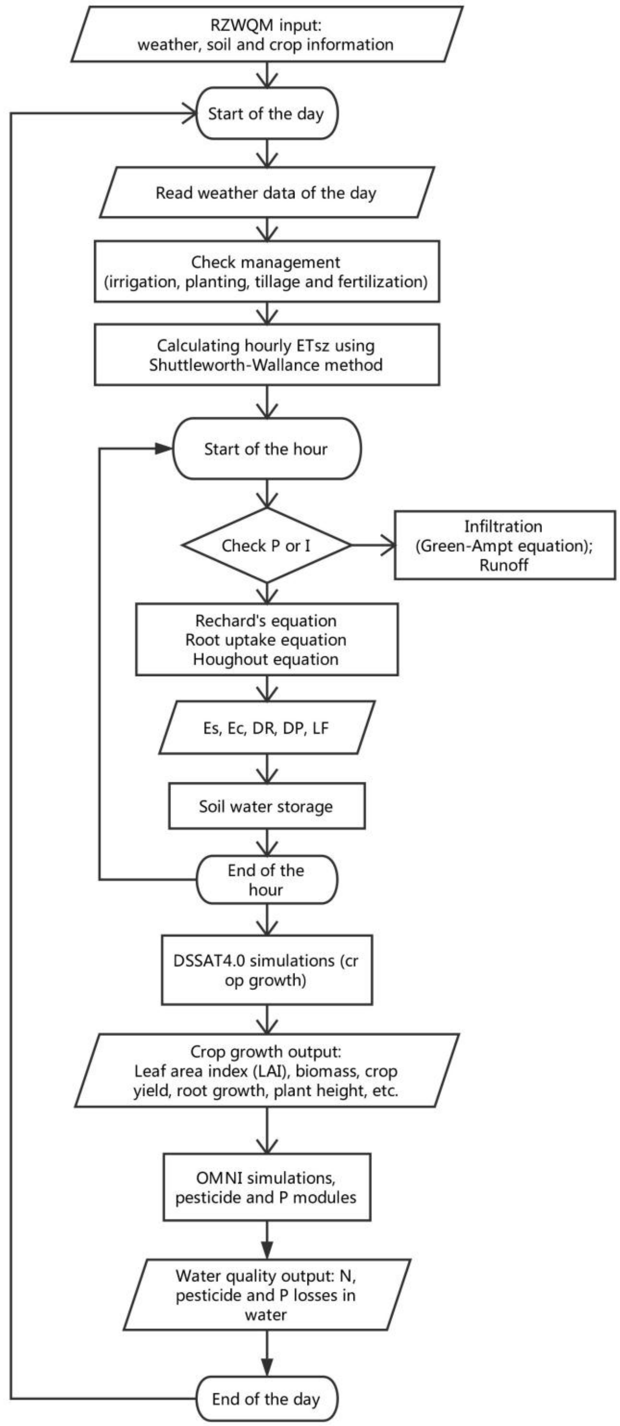

Fig. 2.1. Flow chart of daily and hourly executions of RZWQM (adapted from Fang et al., 2014a), E_s is soil water evaporation; E_c is crop transpiration; ET_{sz} is reference evapotranspiration; DP is deep seepage; DR is drainage; LF is lateral flow; P is precipitation; and I is irrigation.

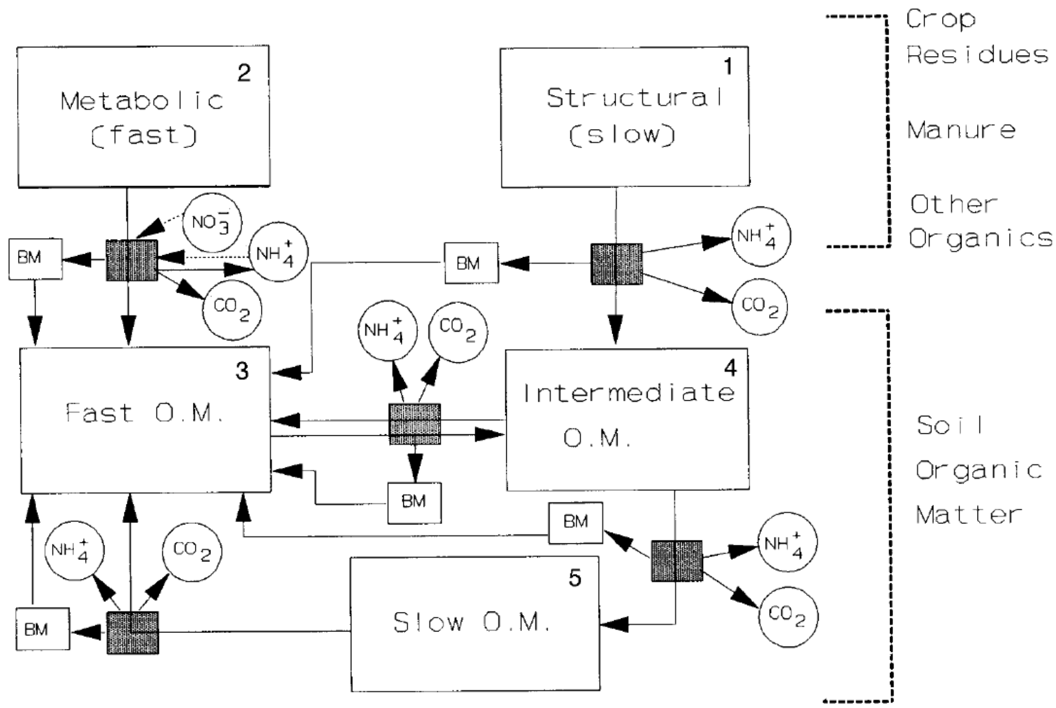

Figure 2.2. Aerobic decay of organic matter in OMNI submodel (adapted from Ahuja et al, 2000).

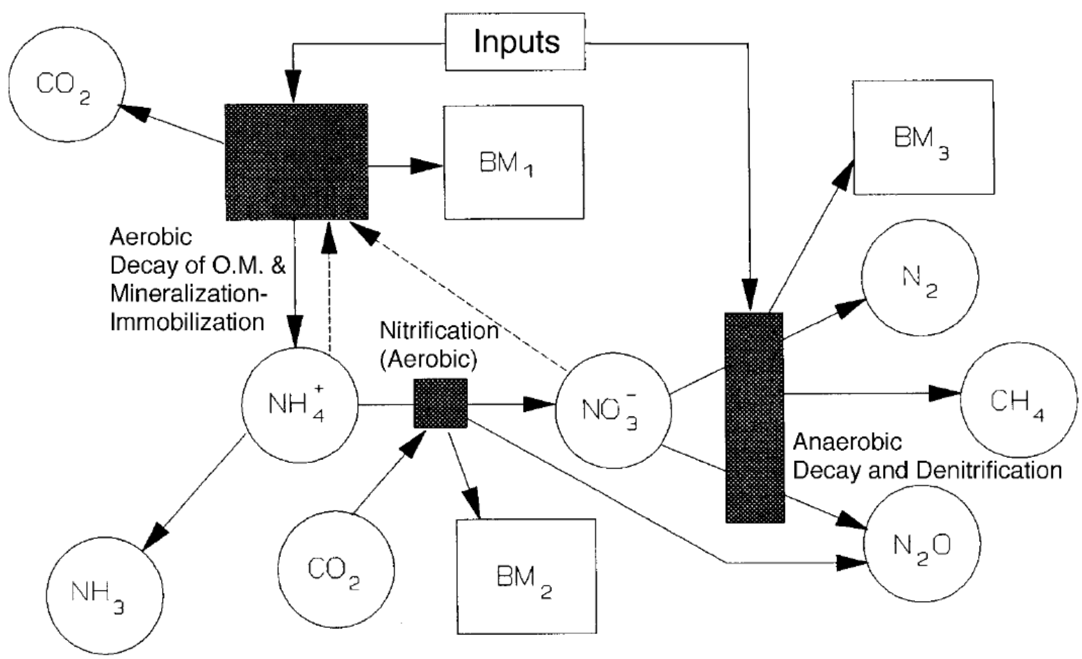

Figure 2.3. Aerobic and anaerobic processes in OMNI submodel (adapted from Ahuja et al, 2000).

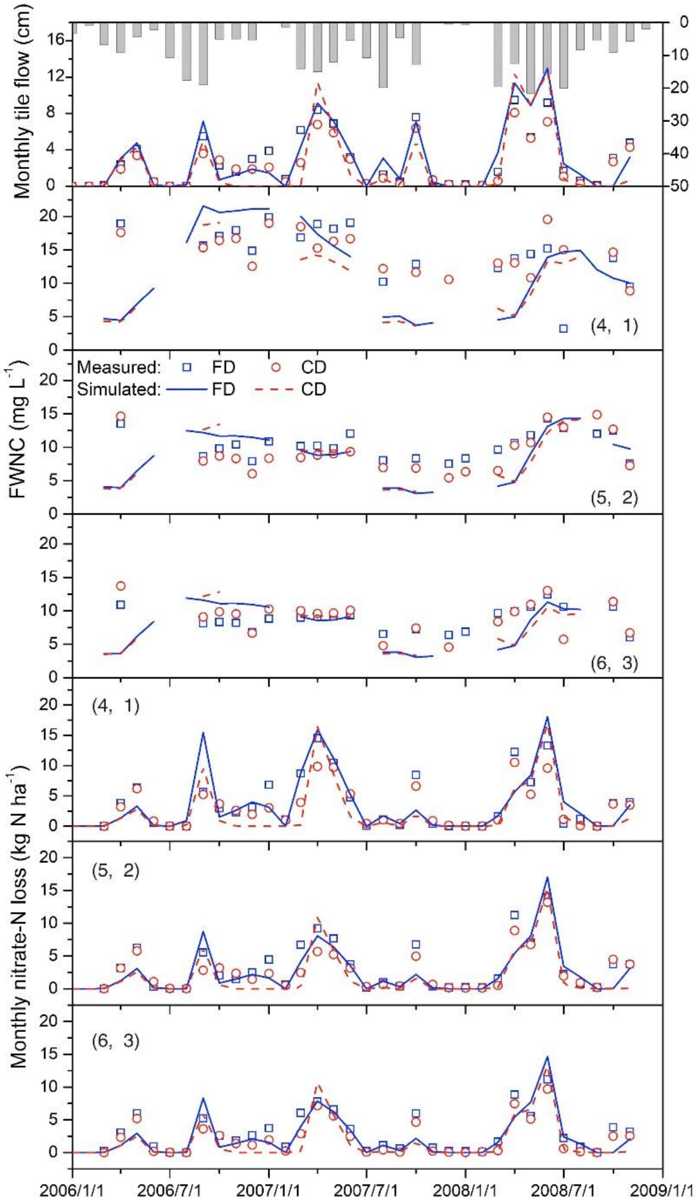

Fig. 2.4. Measured and simulated monthly tile flow, flow weighted nitrate-N concentration (FWNC), and nitrate-N losses. These are averaged from plots 4, 5, 6 under free drainage (FD: 2006–2008) and from plots 1, 2, 3 under controlled drainage (CD: 2006–2008) conditions. For FWNC, some of the measured and simulated data with low tile flow were removed due to low impact on simulated and measured N loss; plot numbers are shown in brackets (adapted from Fang et al., 2012).

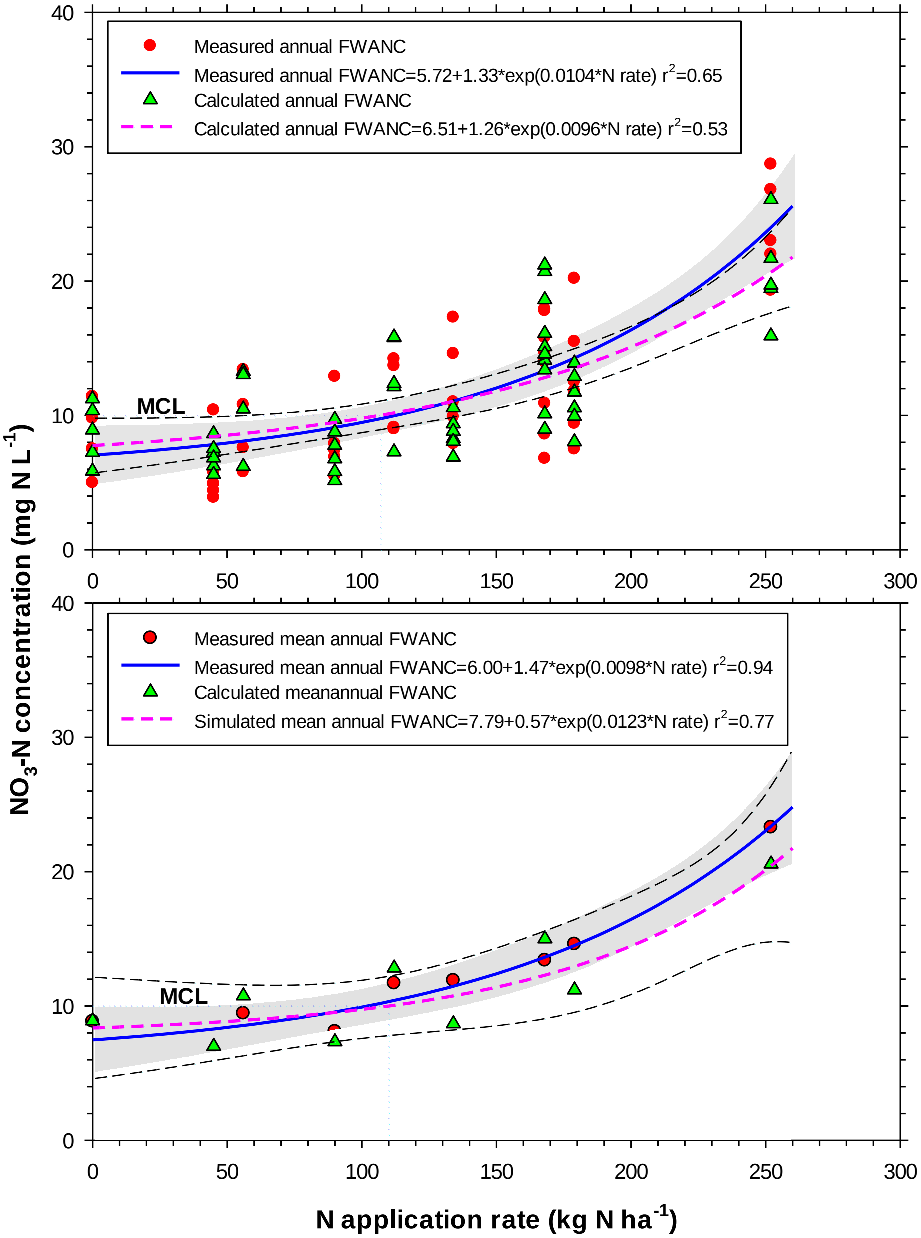

Fig. 2.5. Measured and simulated NO3-N concentration at different N rates and their fitted curves using data a) in individual year and b) average across years. The shaded areas are within the 95% confidence interval for the fitted curves based on the simulated values. The thinner short dash lines are the upper and lower boundary of 95% of confidence interval for the fitted curves based on the simulated values. FWANC, flow-weighted average NO3-N concentration (mg N L^{-1}); MCL, maximum contaminant level (adapted from Qi et al., 2012).

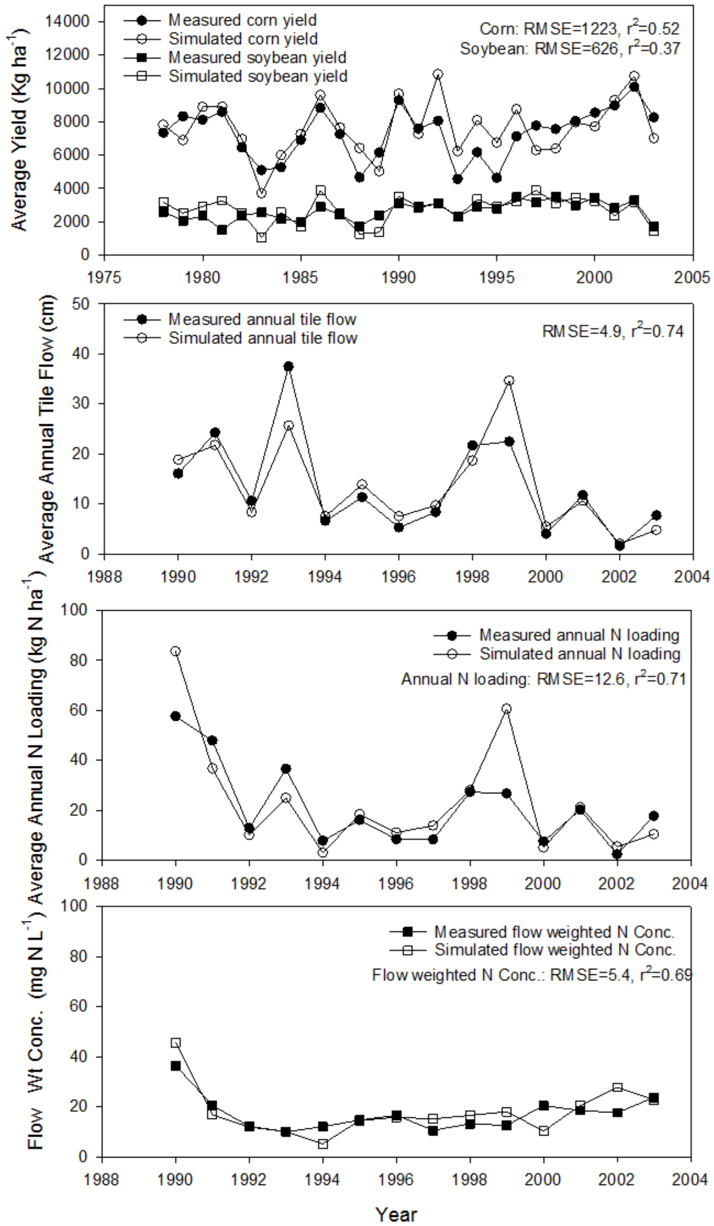

Figure 2.6. Simulated and measured average corn and soybean grain yield, yearly tile flow, yearly N loading in tile flow, and flow weighted N concentration in tile flow across all treatments (adapted from Ma et al., 2007c).

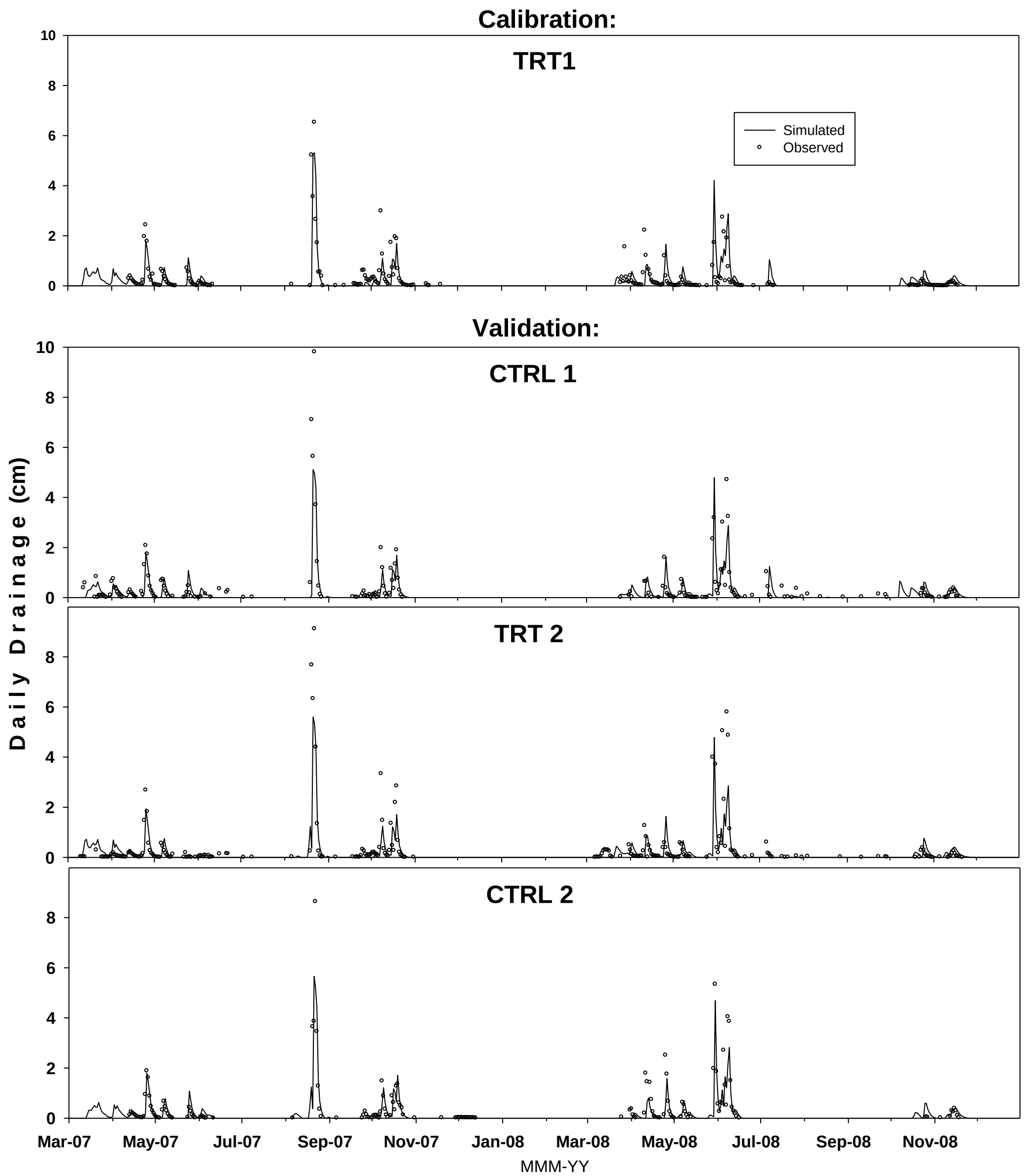

Figure 2.7. Measured and simulated daily drainage in 2007 and 2008. Daily drainage in 2006 was minor after the daily drainage measurement starting date of 12 April 2006. TRT1: winter rye growth prior to corn in odd years and prior to soybean in even years; TRT2: winter rye cover crop growth prior to soybean in odd years and prior to corn in even years; CTRL1: corn in odd years and soybean in even years without cover crop, and CTRL2: soybean in odd years and corn in even years without cover crop (adapted from Qi et al., 2011).

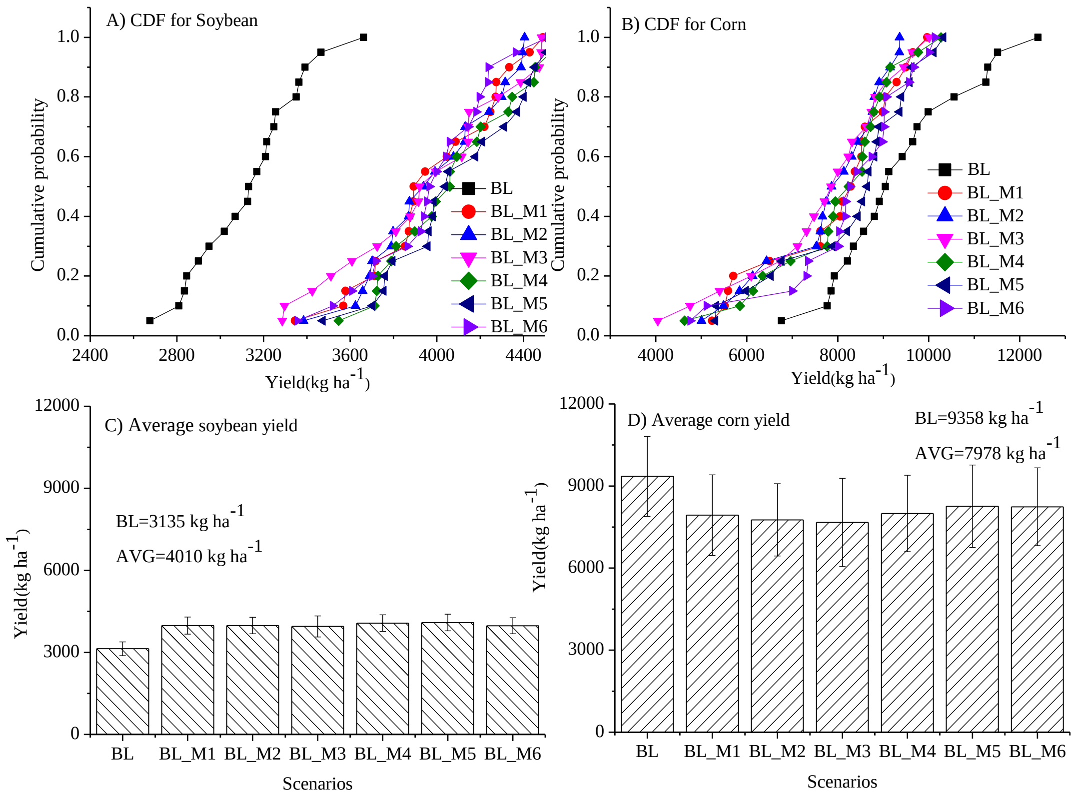

Figure 2.8. **Cumulative distribution functions (CDFs) of soybean and corn grain yields for future under different scenarios: a CDFs of soybean yields; b CDFs of corn yields; c soybean yields for different models; d corn yields for different models. BL: the baseline; BL_M1 to BL_M6: future scenarios from different climate models; AVG: average over six models (adapted from Wang et.al., 2015).**

Table 2.1. The statistics for model evaluation (C_i and M_i are the model calculated and experimental measured points, n is the number of observations, $\bar{C}$ and $\bar{M}$ are the average calculated and measured values), Adapted from (Ma et al., 2012).

Statistics	Satisfactory range	Full name	Equation
PBIAS	-15 % <PBIAS <15%	Percent bias	$\text{PBIAS} = \frac{\sum_{i=1}^{n}(M_i - C_i)100}{\sum_{i=1}^{n} M_i}$
NSE	>0.7	Nash-Sutcliffe model efficiency (Moriasi et al., 2007)	$\text{NSE} = 1 - \frac{\sum_{i=1}^{n}(M_i - C_i)^2}{\sum_{i=1}^{n}(M_i - \bar{M})^2}$
IoA	>0.7	Index of Agreement (Willmott, 1981)	$\text{IoA} = 1 - \frac{\sum_{i=1}^{n}(C_i - M_i)^2}{\sum_{i=1}^{n}(\lvert C_i - \bar{C}\rvert + \lvert M_i - \bar{M}\rvert)^2}$
RMSE	-	Root Mean Square Error	$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(C_i - M_i)^2}{n}}$
RRMSE	<30%	Relative RMSE	$\text{RRMSE} = \frac{RMSE}{\bar{M}}$
r^2	> 0.80	Coefficient of determination	$r^2 = 1 - \frac{\sum_{i=1}^{n}(M_i - \bar{M})(C_i - \bar{C})^2}{\sum_{i=1}^{n}(M_i - \bar{M})^2 \sum_{i=1}^{n}(C_i - \bar{C})^2}$
RSR	⩽0.7	RMSE-observations standard deviation ratio	$\text{RSR} = \frac{RMSE}{STDEV_{obs}} = \frac{\sqrt{\sum_{i=1}^{n}(M_i - C_i)^2}}{\sqrt{\sum_{i=1}^{n}(M_i - \bar{M})^2}}$

Table 2.2. Choice of hydraulic parameters and variables to be considered for calibration for hydrology processes or outcomes (adapted from Ma et al., 2011).

Processes or Outcomes	Related Parameters or Variables
Soil water dynamics	Brooks-Corey parameters, especially $\theta_{1/3}$ (1/3 bar) and θ_{15} (15 bar suction), pore size distribution index (λ), bubbling pressure (h_b), N_2, and K_{sat}, bulk density or porosity, water inputs to the soil and losses from the soil including plant water uptake.
Runoff	K_{sat} at surface layer, rainfall intensity, presence of macropore flow, and surface crusting.
Tile flow	K_{sat} and lateral K_{sat}, tile spacing and depth, lateral flow below tile controlled by a lateral hydraulic gradient, drainable porosity (porosity – $\theta_{1/3}$) and water table leakage rate.
Water table fluctuation	K_{sat} at lower soil layers, tile flow amount, lateral flow below the tile lines, and leakage rate.
ET_{rs}	Albedo, residue cover, LAI (leaf area index) simulation, stomatal resistance, soil surface resistance to vapor flux, and rooting depth.
Water uptake	ET_r, rooting depth, soil water content, $\theta_{1/3}$ and θ_{15}, K_{sat} by layer, and soil root growth factor (SRGF).

Table 2.3. Examples related to drainage component and drainage water quality calibration in RZWQM (adapted from Ma et al., 2011).

Parameters Calibrated	Measurements to Match	Authors
Interpool transfer coefficients among soil carbon pools	N loss in tile flow, soil N distribution	Malone et al. (2010) and Ma et al. (1998)
Lateral hydraulic gradients and lateral hydraulic conductivity, Brooks-Corey soil water retention parameters	Tile flow	Malone et al. (2010), Ma et al., (2007c), Nolan et al. (2011), and Qi et al. (2011)
Porosity and field capacity	Subsurface drainage	Kumar et al. (1998a) and Bakhsh et al. (2004a)
Pesticide adsorption constant and pesticide half-life	Pesticide loss in tile drainage	Bakhsh et al. (2004b)
Lateral sorptivity factor to macropore walls	Pesticide leaching into tile flow	Kumar et al. (1998a) and Malone et al. (2001)
Initial soil water content if not measured	Pesticide soil distribution, tile flow	Azevedo et al. (1997) and Singh et al. (1996)
Brooks and Corey fitting parameters, K_{sat}, lateral K_{sat} and drainable porosity	tile flow	Ahmed et al. (2007a)

Connecting text to Chapter 3

Chapter 2 introduced the RZWQM by presenting the development and improvement of its hydrologic and GHG emission components, the theories used for computing the water balance and GHG emissions, the model parameterization approaches, previous works on model evaluation and its comparisons with other models, model applications to assess agricultural management and climate change impacts on hydrology, crop growth and water quality, model limitations and future work. Chapter 3 presents the first attempt of evaluating the hydrologic component of RZWQM2 (Root Zone Water Quality Model) using a comprehensive hydrological dataset including subsurface tile drainage, subirrigation, soil water content, sap flow and crop growth data (leaf area index, crop yield and crop growth stages). A Kalman filter technique was applied to enhance model reliability and reduce predictive uncertainties.

The following manuscript, co-authored by Dr. Zhiming Qi, Chandra A. Madramootoo, and Ajay K. Singh, has been published in the journal of Computers and Electronics in Agriculture.

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Chapter 3

Simulating hydrologic cycle and crop production in a subsurface drained and sub-irrigated field in Southern Quebec using RZWQM2

Qianjing Jiang, Zhiming Qi, Chandra A. Madramootoo, Ajay K. Singh

Abstract

Agricultural system models are promising tools in evaluating the agro-environmental effects of water management practices. However, very few models have been tested using a comprehensive hydrologic data set. The present study's objective was to evaluate the hydrologic component of RZWQM2 (Root Zone Water Quality Model) using a comprehensive hydrological dataset including subsurface tile drainage, subirrigation, soil water content, sap flow and crop growth data such as leaf area index, crop yield and crop growth stages. Drawing on 2008 and 2009 data from a farm site in Southern Quebec, the RZWQM2 model showed accurate simulation in soil water content, sap flow, growth stage, leaf area index, and crop yield. While mean values for growing season tile flow under both free drainage (FD) and controlled drainage with subirrigation (CD-SI) were reasonably accurate, winter tile flow was significantly overestimated, indicating RZWQM2's reliability to be compromised by its imperfect winter drainage process. Accordingly, a Kalman filter technique was applied to enhance model reliability and reduce predictive uncertainties. A novel modelling approach, RZWQM2 model equipped with a Kalman filter algorithm adequately simulated, in both calibration and validation phases, the hydrology and corn growth which occurred under both FD and CD-SI systems at the selected field site. Simulation results suggest that RZWQM2 model can be used for water management under subsurface drained and irrigated field and the Kalman filter technique significantly improved the accuracy of RZWQM2 model in simulating winter drainage in cold areas.

3.1 Introduction

For agricultural crops, both excesses and penuries of water can result in irreversible crop damage and attending yield losses. A key water management practice in removing excess water from agricultural soils in humid regions, artificial drainage has been widely installed in the humid and cold climate regions of the U.S. Midwest and Northeast (Ritter et al., 1995), as well as eastern Canada (Madramootoo et al., 2007). Regarded as a best management practice (BMP), water table management not only reduces N loss but also increases or maintains crop yield (Madramootoo et al., 2001). Water table depth management through subsurface tile drainage can operate in three ways: free drainage (FD), controlled drainage (CD), or controlled drainage with subirrigation (CD-SI).

Besides the benefits on crop production, CD-SI also provides significant benefits for the environment. A 1998 study conducted at a field site in the St. Lawrence Valley near Montreal, Quebec demonstrated that CD-SI deceased nitrate (NO_3^-) leaching, while degrading NO_3^- in the field and limiting its translocation (Andrade et al., 2002). Further benefits were achieved when dissolved organic carbon is added to the sub-irrigation water, including the acceleration of denitrification rate, reduction of NO_3^- pollution, and lessening of N_2O release attributable to subirrigation-enabled bacterial reduction of N_2O to N_2 (Andrade et al., 2002).

A number of reports over the last few decades have shown CD-SI to increase crop yield while decreasing N and P losses. Controlled drainage reduced drainage outflow and enhanced denitrification, thereby reducing NO_3–N losses (Ridao et al., 1998). The reduction of N and P loss achieved by implementing CD varied from 30% to 50% of losses under FD, depending on soil type, climate, drainage system design and management (Evans et al., 1995). On a sandy loam soil in Southwestern Ontario, Canada, one year's tomato (*Solanum lycopersicum L.*) yield under a CD-SI system increased 11% over that achieved under FD, while another year's corn (Zea mays L.) increased by 64% under the same comparison. Meanwhile, the total NO_3^- loss under the CD-SI system was 24% lower than under the FD system (Tan et al., 1997). Field study conducted in an experimental site in Southern Quebec from 2001 to 2002 also indicated significant improvement of corn yield which is around 35% under CD-SI than FD (Stampfli and Madramootoo, 2006). A two-year field study conducted on a loamy sand in Sweden showed that under CD, NO_3^- losses to subsurface drainage in the first and second year were 78% and 94% less than under FD, while the equivalent reductions in phosphorous losses were 58% and 85% (Wesstrom et al., 2001). On a silty clay loam soil in Iowa, annual NO_3^- losses from 2007 to 2010 were reduced by 36% under CD compared to FD (Helmers et al. (2012). In another study, the increase in crop N uptake and yield observed under a CD (vs. FD) system was attributed to a lack of water stress during the growing season and the resulting higher N and P use efficiency (Wesström et al., 2014).

Though these field studies undertook to compare drainage flow rates, water quality, and crop yield under CD or CD-SI systems to those under standard FD practices, evaluation of the CD and CD-SI system's performance remained limited and the data limited to a few years under specific weather and soil conditions. Moreover, field experiments are time consuming and prohibitively costly. However, agricultural system models are promising tools to evaluate different drainage systems over a long period of time for locations differing in soil type and climatic conditions (Thorp et al., 2007b). For example, the RZWQM2 can be executed for over a hundred years to evaluate long term impact of agricultural management and climate change on crop production and water quality.

Over recent decades, the Root Zone Water Quality Model's ability to investigate agricultural management practices' effects on water quality and crop growth for sites differing significantly in their climatic and pedological conditions, has been widely evaluated (Ma et al., 2012). The model's latest version (RZWQM2) incorporates the DSSAT V4.0 crop growth models and the SHAW energy balance model (Ma et al., 2011). Akhand et al. (2003) successfully used RZWQM to predict water table, subsurface drainage, and soil moisture in agricultural fields situated in Nova Scotia and Southern Ontario, Canada. The model's prediction of tile drainage and leached NO_3^- for sites in Iowa and the Georgia Piedmont was evaluated and shown to be accurate (Singh et al., 1996; Bakhsh et al., 2001; Abrahamson et al., 2006; Saseendran et al., 2007; Qi et al., 2011, 2012). Lu (2015) first tested the performance of RZWQM2 in predicting the surface runoff and drainage in a subsurface drained field in Ontario and found that the model satisfactorily simulated surface runoff and subsurface drainage in FD field but for the CD-SI field the simulation was not acceptable.

With the exception of a study using DRAINMOD (Morrison et al., 2014), few studies have evaluated the performance of field-scale agricultural drainage models, drawing on a full set of hydrological data, in simulating hydrology in regions subject to extreme cold and humid conditions (i.e., Southern Quebec, Canada). For instance, DRAINMOD has been evaluated on the basis of its capacity to accurately simulate measured runoff, subsurface drainage flow, erosion, and sediment-bound nitrogen data (Wright et al., 1992), drainage and water table (Dayyani et al., 2010a, b; Skaggs et al., 2012; Golmohammadi et al., 2016), drainage and crop yield (Luo et al., 2009), or drainage only (Singh et al., 1996), but rarely against a full set of hydrological data including both ET and soil water content. The Agricultural Drainage and Pesticide Transport (ADAPT) model was tested against measured subsurface drainage and runoff

(Chung et al., 1992) and subsurface drainage flow only (Sogbedji and McIsaac, 2002; Gowda et al., 2012), while RZWQM has been evaluated using water table, soil water storage, tile drainage, N balance, and crop yield and biomass (Ma et al., 2007c), but none of the models have been assessed using ET data measured under drainage conditions.

In calibrating a hydrologic model for simulating only one or two observed agricultural system components, modelers may ignore simulation errors with respect to further unmeasured hydrologic components, thereby erroneously presenting the overall simulation performance as accurate. However, it may in fact provide a poor simulation of important non-quantified hydrological components. For instance, one can decrease the evapotranspiration (ET), which was not monitored, to obtain a highly accurate simulated drainage; however, the ET value with which the model operates may deviate significantly from its genuine value in the field. No previous study has been conducted to evaluate agricultural models with a comprehensive dataset.

The objectives of this study are to evaluate RZWQM2 for a site in Southern Quebec implementing both FD and CD-SI systems, using a comprehensive dataset including subsurface drainage flow, crop transpiration, soil water content, as well as crop yield, leaf area index and growth stages. A model calibration strategy to further minimize the error between simulated vs. measured drainage by including a Kalman filter system into the model was tested. Although the Kalman filter technique has been extensively studied and successfully applied in assimilating measurements and data (de Wit and van Diepen, 2007; Flores et al., 2012; Zhao et al., 2013), few studies have evaluated its performance in modeling and model calibration (Clark et al., 2008). In this paper, the accuracy of a drainage estimation system implementing a Kalman filter and drawing on a dataset from a field in Southern Quebec was evaluated.

3.2 Materials and methods

3.2.1. Field experiment

The field study was conducted from 2008 to 2009 at a 4.2 ha subsurface drained corn field near St. Emmanuel, Quebec (latitude 45.32, longitude −74.17). The soil at this site is a Soulanges very fine sandy loam with 50 g kg^{-1} organic matter in the top layer (0–0.25 m), followed by layers of sand clay loam with 1.5% organic matter (0.25–0.55 m) and clay layers with little organic matter content (0.55–1.0 m). Corn was planted in both years at a row spacing of 0.76 m. In 2008 *Mycogen* seed was planted on May 4 at a density of 89,000 seeds ha^{-1}, and in 2009 *Pioneer 38N88* was planted on May 7 at a seeding rate of 85,000 seeds ha^{-1}.

Subsurface drained plots (75 m × 15 m) were grouped in three blocks, each housing two water table management regimes (FD and CD-SI) with three N application rates nested within each water table management regime (Fig. 3.1). The water table management practices were: conventional free drainage (FD) and controlled drainage with subirrigation (CD-SI), running along the direction of drainage pipes in each of the blocks. The three N applications were set up orthogonally in the middle two strips of each block. The subsurface drains were installed at a depth of 1.0 m on a 0.5% slope in the center of each plot (Madramootoo et al., 2001). For CD-SI the water table depth was set at 0.6 m and 0.75 m in 2008 and 2009, respectively. The three N applications, low N, medium N and high N, and N application timing are listed in Table 3.1. Subirrigation was achieved by pumping water from a well into the drainage pipes through water table control structures. Controlled drainage in sub-irrigation plots was initiated on May 21 and ended on Sept 9 in 2008, while in 2009 it began on June 23 and ended on Sept 9.

3.2.2. Data collection

A weather station was installed in situ to measure hourly temperature, precipitation, relative humidity, wind speed, solar radiation and soil temperature. Missing readings for some days (e.g. for precipitation) were drawn from the Environment Canada weather station at Côteau-du-Lac (Station ID – 7011947), located 500 m from the experimental site. Soil properties, including soil texture, organic matter content and bulk density were measured using undisturbed soil cores sampled from the field.

Available experimental measurements included subsurface drainage flow, subirrigation amount, water table depth, soil water content (θ), crop transpiration (sap flow), grain yield, leaf area index (LAI), and phenological dates for emergence, silking and physiological maturity. The LAI was measured from June 10 to July 30 in 2008 using a LI-3000 (LI-COR Environmental, Lincoln, NE) and from July 21 to Aug 21 in 2009 using a LI-2000. The LAI was measured six times during the 2008 growing season, starting from an early stage on June 10 to a peak growing stage on July 30, and five times from July 21st to September 7th in 2009. The observed physiological maturity dates were Sep 21, 2008 and Sept 24, 2009 and the harvest dates were Oct 15, 2008 and Oct 20, 2009. In the two control stations, 12 (2 plot drains × 2 drainage treatments × 3 blocks) tipping bucket flow meters were installed to measure subsurface drainage flow, one for each drainage pipe. The flow meters were calibrated and connected to a data logger (Tait et al., 1995). The θ was recorded with two sets of soil moisture sensors: WATERMARK sensors (Model No. 6450; Spectrum technologies, Inc., Plainfield, Ill, USA) installed at a depth of 0.15 m, and ThetaProbe sensors (Model ML2x; Delta-T Devices Ltd., Cambridge, UK) at a depth of 0.45 m (Singh, 2013). Observed θ data is available for a depth range of 0.20–0.25 m in 2008 and 0.40–0.45 m in 2009. Corn transpiration was measured by a sap flow method using a Dynagage Flow32-1K system (Dynamax, Houston, Texas, USA). Mean diameter of the corn stem was 22 and 23 mm in 2008 and 2009, respectively. Eighteen gage models (one gage for each plot) of SGB19-ws (diameter ranging from 18 to 23 mm) and SGB25-ws (diameter ranging from 24 to 32 mm) from Dynagage Flow32-1K system (Dynamax Inc, Houston, Texas, USA) were installed on 22 July 2008 and 22 July 2009 to measure the sap flow of three plants in each plot. The gages installed on the stem were connected to data logger with 20 to 24 gage cables, and the sap flow readings were taken every 60 s and averaged over 30 min intervals.

3.2.3. Overview of RZWQM2

The RZWQM is aone-dimensional agricultural system model that houses physical, chemical, and biological processes for simulating the movement of water, nutrients, and pesticides, as well as crop growth in the field under various management practices (Ahuja et al., 2000b). The model uses the Green-Ampt equation (Green and Ampt, 1911) to simulate the infiltration of surface water and melted snow into the soil and the Richards equation (Richards, 1931) to calculate water distribution in the soil profile between rainfall or irrigation events (Ahuja et al., 2000b). The potential evaporation and crop transpiration are described by the Shuttleworth-Wallace equation (Shuttleworth and Wallace, 1985). Tile drainage flux is calculated by the Hooghoudt equation (Ahuja et al., 2000b). Agricultural management practices option available for users include crop cultivar selection and planting, manure application, irrigation, fertilization, pesticides and tillage. In case of subirrigation, water was introduced to the soil profile at a user-defined depth as a source for solving Richards equation (Richards, 1931).

3.2.3.1. RZWQM2 model calibration

The model was calibrated and validated against two years of field experiment data (2008 and 2009). Calibration was based on phenology of corn growth stages, leaf area index (LAI), drainage flow rate, corn transpiration, soil water content, water table depth and yield in FD plots, and measured data in CD-SI plots were used to validate the model.

i. Hydrology component

The bulk density was measured before planting in 2008. Soil hydraulic parameters including saturated and residual soil water content, saturated hydraulic conductivity (k_{sat}), lateral k_{sat}, bubbling pressure and pore size distribution were calibrated first, using measured soil moisture content and subsequently adjusted using drainage flow data. Both increasing the bubbling pressure and decreasing the pore size distribution will result in more water remaining in the soil, thereby decreasing the movement of water downward into the drains (Walker et al., 2000). To maintain a high water table, the k_{sat} of the last soil layer was set at 0.1 mm h^{-1} (Thorp et al., 2007b). The lateral K_{sat} was suggested to be adjusted as 2 times of vertical K_{sat} to match the peak drainage flow (Qi et al., 2011). Soil root growth factors (SRGF), representative of the ability of crop roots to grow in a given soil layer, influence the amount of soil water which roots can potentially take up from this layer (Ma et al., 2009). The SRGF values for corn were adopted from Qi et al. (2011). Detailed soil hydraulic parameters are shown in Table 3.2.

In RZWQM2, potential evapotranspiration (ET_p) is estimated using the Suttleworth-Wallace approach (Ahuja et al., 2000b). To simulate the ET_p, a number of parameters are needed, including daily leaf area index (LAI), surface soil resistance, minimum stomatal resistance and the albedos of dry soil, wet soil, crop and fresh residue (Ma et al., 2011). A reasonable simulation of LAI is essential for correct ET_p simulation; therefore, given that LAI is closely related to the crop growth stage, accurate simulation of LAI requires an accurate knowledge of crop phenology. Surface soil resistance in the Shuttleworth-Wallace equation is sensitive to soil evaporation; therefore, increasing the albedo of bare dry soil or bare wet soil would lead to a decrease in evaporation. Similarly, increasing the crop's albedo at maturity would result in lower transpiration. Detailed calibrated parameters are listed in Table 3.3.

ii. Nutrient component

To properly initialize the soil microbial populations, it is suggested to run the model for at least 10–12 years prior to the simulation period (Ma et al., 1998). Accordingly, the model was run from 1998 to 2007 to stabilize the organic matter pools. Corn was planted using the same cultivar as 2008 and 2009, The weather information from 1998 to 2009 was obtained from the weather station at Côteau-du-Lac. Corn was planted continuously within the 10 years using the same cultivar parameters as indicated in Table 3.4 and the field was freely drained with the N fertilization amount at 180 kg ha^{-1} per year. Other agricultural management applied was the same as the treatment in 2008 and 2009, including the timing of crop planting and harvest, tillage, and fertilization. Initial soil organic matter (SOM) was obtained from the field experiment and the OM fraction were set at 4%, 3%, 2% and 2% in the soil layer at depths of 0.20, 0.40, 0.60 and 0.80 m, respectively.

The nutrient parameters were calibrated to obtain reasonable crop yields. The 2009 simulated corn yield was roughly 4.0 Mg ha^{-1} with RZWQM2 default nutrient parameters, whereas the observed yield was over 10 Mg ha^{-1}. In view of this mismatch, model output was found to show unreasonably low mineralization (around 20 kg N ha^{-1} y^{-1} for the top 0.80 m of soil). According to a soil measurement made near Montreal in 2001, where a 50 kg N ha^{-1} fertilizer application was made, potential N mineralization in the top soil (0–0.20 cm) varied between 64 and 122 kg ha^{-1}, according to the soil texture (Simard et al., 2001). Carpenter-Boggs et al. (2000) reported the mineralization amount from 150 to 160 kg N ha^{-1} during the growing season with 181 kg N ha^{-1} fertilization in South Dakota, US. The simulated mineralization being too low, more C needed to be portioned to the fast or intermediate pools (Ma et al., 2011). Accordingly, the interpool transformation coefficient for the slow residue pool to intermediate soil humus pool was adjusted from a default value 0.1 to 0.3, and the fast residue pool to fast soil humus pool transformation coefficient was increased from 0.1 to 0.6 (Thorp et al., 2007b). The death rate of anaerobic heterotrophs was adjusted from 3.4×10^{-33} to 5×10^{-33} and that of aerobic heterotrophs from 5.0×10^{-35} to 4.0×10^{-37} (Table 3.3). These adjustments increased N mineralization from 20 kg ha^{-1} to around 150 kg ha^{-1}. The concentration of NO_3-N in rainwater was set to 1.2 mg L^{-1} based on an analysis of rainwater quality in Montreal (Poissant et al., 1994).

iii. Phenology dates for corn growth stages

In order to accurately simulate the development and growth of crops, crop parameters should be calibrated first against phenological dates, given their effect on crop yield, and secondly against plants' varying sensitivity to water, nitrogen, and temperature stresses at different growth stages (Ma et al., 2011). Since neither the *Mycogen 2R426* nor *Pioneer 38N88* cultivar was included in the DSSAT cultivar database, based on the strategy suggested by Ma et al. (2011), *Pioneer 3382* was selected as the cultivar having predicted phenological dates (emergency, anthesis, and maturity) closest to observed dates. Eight cultivar parameters in the RZWQM2 interface can be used to adjust the growth and development of maize, including P1, P2, P5, G2, G3, PHINT, Maximum plant height at maturity (cm) and Plant biomass at half of maximum height (g), as defined in Table 3.4. The phenological parameters were set to very low values to match the observed growing days, including the days of emergence, silking and maturity. Given the date-of-anthesis' sensitivity to P1 and P2 values, P1 was set at 200 growing degree days (GDD) and P2 was adjusted to 0.3 to match the observed silking day (July 30, 2008 and August 2, 2009). To match the early maturity date of Sep 21, 2008, P5 was initially set as low as 550 GDD, despite the acceptable range being between 600 and 1000 GGD. However, it led to the underestimation of corn yield, thus P5 was adjusted to 610 GGD to achieve a more reasonable estimation of both yield and maturity date. The value of PHINT was adjusted to match LAI during the vegetative periods. Both G2 and G3 were set to high values in the range to correctly simulate corn yield.

iv. Kalman filter

The current RZWQM2 model predicted reasonable mean values for tile flow under FD in the growing season, while θ, water table depth, sap flow, growth stage, LAI, and crop yield showed a percent bias (PBIAS) within ±15%. However, the mean tile flow under CD-SI, as well as tile flow under FD in winter, were significantly overestimated.

Given the considerable discrepancy (i.e., poor correlation) between simulated and observed values, one or more factors within the model, responsible for generating the error, must be identified and appropriately adjusted. The Kalman filter is an effective and widely-used method to eliminate errors which fits the Gaussian model (Xie and Zhang, 2010). Therefore, the errors which fit the Gaussian model would be eliminated if the RZWQM2 model were calibrated by the Kalman filter (Camporese et al., 2009). Hence, the Kalman filter is a promising approach for error elimination in this study.

In applying the Kalman filter, the variance between model simulations and observed measurements is used to quantify model error (Clark et al., 2008). The characteristics and parameters of the Kalman filter having been obtained, it can be used to calibrate the model and optimize simulation results.

At the onset, the Hooghoudt steady state equation serves to compute drainage flux in the RZWQM2 model:

$$df = \frac{8K_e d_e m + 4K_e m^2}{L^2} \quad [3.1]$$

d_e is the equivalent depth of the impermeable layer below the tile drains (as affected by drain depth and midpoint water table height; mm),

df is the drainage flux ($mm\ h^{-1}$);

m is the midpoint water table height above the drain (mm);

K_e is the effective lateral saturated hydraulic conductivity ($mm\ h^{-1}$); and

L is the distance between drains (mm);

The drainage flux model could be presented as the linear system (Sinopoli et al., 2004):

$$\hat{x}_{\bar{k}} = Ax_{k-1} + Bu_{k-1} + q_{k-1} \quad [3.2]$$

$$y_k = Hx_k + r_k \quad [3.3]$$

such that:

$$\sum_{i=1}^{i=k} x_i = \sum_{i=1}^{1=k} df_i = \sum_{i=1}^{i=k} \frac{8K_{e_i} d_{e_i} m_i + 4K_{e_i} m_i^2}{L_i^2} \quad [3.4]$$

where,

$\hat{x}_{\bar{k}}$ is the predicted state of the system at day *k;*

x_{k-1} is the state of the system (the accumulated simulated from day 1 to day *k*-1);

u_{k-1} is the control signal (*i.e.*, observed drainage) of the system at day *k*-1;

q_{k-1} is the system error of designed linear system at day *k*-1;

A and *B* are the linear system's parameter;

y_k is the observed value at day *k;*

r_k is the error of observation, *i.e.*, the daily error between simulated and observed values; and

H is the system's measurement parameter, in this study $H = 1$.

The values of system parameters A and B are the transition matrix and the control matrix, respectively (Roweis and Ghahramani, 1999), which are determined by the dimension, order and relationship of the linear system's different variables. For example, in the present study, having only one input and one output, so A and B are matrix with only one unit (a 1×1 matrix). As the simulated drainage is of the same order as the control input, the values of A and B must be real numbers. The accumulated drainage at day k represents the sum of accumulated drainage at day k-1 along with the control input; accordingly, the values of A and B are both 1.

The specific sequence of the use of a Kalman filter in this study is summarized in Fig. 3.2. The FD data served as initial data, which could then be expressed in the form of the linear system model. A Kalman filter then being applied, all the necessary variables and parameters could be obtained. A best estimation could be generated after optimization of the Kalman filter.

The Kalman filter system applied in the present study consisted of five main steps: the first two leading to an updating of time history variables, while the last three steps updated current state variables (Mehra, 1970). Detailed information for the five steps are as follows:

Step 1. Predict simulated drainage and calculate system error at day k.

Based on the linear system (Eq. [3.2]), the simulation value on the current day (k) could be predicted by the simulation value and control signal of the previous day (k − 1) as well as the previous day's system error. This predicted value would be modified in Step 4.

Step 2. Predict the estimation error at day k.

The estimation error at day k, $P_{\bar{k}}$, is given as:

$$P_{\bar{k}} = AP_{k-1}A^T + Q \quad [3.5]$$

where, A is the system parameter, P_{k-1} is the estimation error at day k-1, T stands for matrix transpose, Q is the variance of the system error q_k.

Based on the linear system given above (Eqs. [3.2] and [3.3]), the estimation error of the current moment could be predicted by the system parameters and the true error of the last moment. Obviously, the estimation error is not the real error and it would be updated by the Kalman gain and other system parameters in step 4.

Through the linear system designed above, the two state variables of the Kalman filter were predicted and updated in the time history.

Step 3. Determine the Kalman gain at day k.

The Kalman gain is the most important coefficient of the Kalman filter, allowing updating of both the best estimation value and the true error. The Kalman gain on the current day k (K_k) is given as:

$$K_k = \frac{P_{\bar{k}}H^T}{HP_{\bar{k}}H^T + R} \quad [3.6]$$

where, R is the variance of the observation error r_k.

Step 4. Update the estimation value of the system at day k.

With the Kalman gain generated in step 3 ([3.6]), the simulated value can be revised to a best estimate value for the current moment, *i.e.*, the final simulated result.

$$\hat{x}_k = \hat{x}_{\bar{k}} + K_k\left(y_k - H\hat{x}_{\bar{k}}\right) \quad [3.7]$$

Step 5. Update the estimation error at day k

The last step is to revise the estimation error to the true error using the Kalman gain, thereby preparing for the next round (*i.e.*, day):

$$P_k = P_{\bar{k}}(I - K_k H) \quad [3.8]$$

Where, I is the unit matrix. In the present study, I = 1.

Cycling through the five steps, the Kalman filter algorithm operates automatically one day after another, such that all of the drainage model's Kalman filter parameters and variables are determined day to day. It should be noted that in the present case the Kalman Filter's error was generated from FD data, the function of the Kalman filter having been to eliminate the error associated with a Gaussian distribution. The Kalman filter was then used for both FD and CD-SI data, and the simulation results show that the calibrated model has a good performance. Specific steps and samples of the Kalman filter designed in the present study are presented in the Appendix.

3.2.3.2. Model accuracy statistics

In this study, five statistics were used to evaluate the performance of RZWQM2 in simulating subsurface drain flow, soil water content, crop yield and LAI under different water table management practices and N application rates, in comparison with observed data. They are percent bias (PBIAS), root mean squared error (RMSE), relative RMSE (RRMSE), Nash-Sutcliffe model efficiency (NSE) and index of agreement (IoA). For the NSE and IoA, a value 1 indicates perfect accuracy. Percent bias (PBIAS) measures the difference in mean values between simulated and observed data, and NSE is an indicator of the goodness of fit in terms of variance. Values of PBIAS within ±15%, NSE > 0.7, and IoA > 0.7 represent a satisfactory model performance (Ma et al., 2012). The value of the RRMSE when model estimates perfectly match observed data is 0, and its acceptable range is ±30%.

$$\text{PBIAS} = \frac{\sum_{i=1}^{n}(O_i - P_i)100}{\sum_{i=1}^{n} O_i} \quad [3.9]$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(P_i - O_i)^2}{n}} \quad [3.10]$$

$$\text{RRMSE} = \frac{RMSE}{\bar{O}} \quad [3.11]$$

$$\text{NSE} = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \quad [3.12]$$

$$\text{IoA} = 1 - \frac{\sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(|P_i - \bar{P}| + |O_i - \bar{O}|)^2} \quad [3.13]$$

where,

n is the number of observations;

$\bar{O}$ is the mean observed value;

O_i is the i^{th} observed value;

$\bar{P}$ is the mean predicted (simulated) value, and

P_i is the i^{th} predicted value.

3.3 Results

3.3.1. Hydrology

Annual precipitation at the site, located in Côteau-du-Lac, QC, was 1123 mm in 2008 and 989 mm in 2009, compared to a long-term average (24 years of complete data between 1978 and 2007) of 986 mm. While 2008 showed more precipitation than the long-term average, the growing season was slightly drier than average. In contrast, annual and growing season precipitation in 2009 were both very close to the historical average. Precipitation during the May to September growing seasons of 2008 and 2009 was similar in pattern and quantity (432 mm and 465 mm, respectively), and slightly below the historical average of 474 mm (Singh, 2013).

3.3.1.1. Drainage

The simulated and observed daily tile drainage is plotted in Fig. 3.3, showing that the model performed well in simulating most of the peak flows. However, it over-estimated the drainage flow in March 2009 and under-estimated it in August and September 2008. The monthly drainage during May to October 2008 and April to Oct 2009 is presented in Table 5. For the FD management scenario, the model over-estimated daily subsurface drainage by 30% (67.8 mm) in the calibration phase. Measured drainage across both years (from April 16 to October 27, 2008 and February 25 to November 6, 2009) was 225.8 mm, whereas the simulated total was 293.6 mm. The over-estimation occurred mainly in March and May, and were 69.5 mm and 38.9 mm, respectively for two years in total. The model under-estimated April 2009 drainage by 20.8 cm, perhaps because the model simulates the snow melt too early (all simulated snowmelt occurred before March 11, 2009). Summer drainage (June to August) under FD was under-estimated, especially in 2008 when the simulated annual ET was as high as 612 mm. The summer period ET might have been over-estimated, leading to an under-estimation of drainage flow.

For the CD-SI management scenario, most peak flows were well simulated, but the total drainage flow over 2 years was over-estimated by 43% (160 mm). The over-estimation of drainage occurred in March (80.5 mm) and May (39.6 mm). Table 5 shows the model accuracy statistics comparing simulated daily drainage with observed values. Daily drainage for the two years was over-estimated in all the plots. The model did not simulate daily drainage well, particularly during the snow melt period. The NSE values of daily drainage estimation for both FD and CD-SI were below zero (Table 5), which indicates a prediction of drainage peaks worse than simply taking the mean observed drainage. A high PBIAS also shows an overall over-estimation of drainage flow. By applying the Kalman filter algorithm after calibrating the RZWQM2 model, the daily drainage predictions for both two treatments were improved significantly. The NSEs were increased from subzero values to 0.91 and 0.89 for FD and CD-SI, respectively. The PBIAS was improved from 30% to 9% for FD and reduced from 43% to 15% for CD-SI. The IoA was also increased from 0.60 and 0.66 to 0.97 for both FD and CD-SI. This improvement was mainly the result of error reduction through the application of the Kalman filter. For the FD drainage regime in the calibration phase and the CD-SI drainage regime in both calibration and validation phases, over the period of March to July 2009 the magnitudes of the RZWQM2 and RZWQM2-Kalman errors were quite distinct, the model error having decreased significantly after applying the Kalman filter algorithm (Fig. 3.4).

Model accuracy statistics for monthly drainage, excluding snow melting periods (Table 6), showed simulated subsurface drainage flow to be in good agreement with observed drainage. The performance of RZWQM2 in simulating monthly drainage under the FD treatment can be judged as “satisfactory” (PBIAS = −1.1%, IoA = 0.75), except for a low NSE of only 0.18. In terms of NSE and IoA, the CD-SI drainage regime simulations showed a better agreement between measured and simulated monthly drainage during the growing season (April to October) than for the FD regime. The overall drainage was over-estimated by 25.2% with an overall NSE value of 0.39 under CD-SI. In both calibration and validation phases, implementing the Kalman filter increased the NSE from 0.18 and 0.39 for FD and CD-SI irrigation regimes, to 0.93 for both (Table 6). The Kalman filter algorithm reduced the under-estimation of the total monthly drainage amount during the growing season from 1.1% to 0.4% in FD, and lowered the over-estimation from 25.2% to 9.0% under CD-SI.

3.3.1.2. Soil water content (θ)

RZWQM2 simulated θ was generally in good agreement (|PBIAS| < 15%) with observed θ data, though the NSE and IoA values were not high (Fig. 3.5, Table 3.7). This is widely encountered in soil moisture simulation studies (Fang et al., 2014 a,b). Though the model significantly underestimated some of the extremely high θ peaks under CD-SI in 2008 (July 23, Aug 7 and Aug 19), it over-estimated some peaks in 2009.

3.3.1.3. Corn transpiration

The observed average sap flow during summer (mainly in August) was 3.6–4.4 mm d^{-1} (Fig. 3.6). For all the irrigation regimes, the error in RZWQM2 simulated (vs. measured) transpiration was ±15%; however, NSE values were not in an acceptable range (Table 3.8). As illustrated in Fig. 3.6, the simulated transpiration showed its best agreement with observed sap flow for the medium N fertilization treatment, with a PBIAS within 2%, $0.32 \leqslant$ NSE $\leqslant 0.37$ and $0.69 \leqslant$ IoA $\leqslant 0.78$ (Fig. 3.6, Table 3.8). Among different N application rates, the model showed no differences in simulated transpiration or LAI, whereas the observed sap flow varied between each treatment (Figs. 3.6 and 3.7).

3.3.1.4. Soil water balance

Based on the growing season water balance generated by the RZWQM2 model in the calibration phrase (Table 9), the water supplied by precipitation was not able to fully support the requirements of water usage through crop transpiration and soil evaporation. Accordingly, soil water storage (174 mm and 123 mm at the onset of the 2008 and 2009 growing seasons, respectively) was used to meet these requirements. The low soil water storage in FD at the end of growing season concurred with the deep simulated water table in August and September. For the CD-SI, no significant increase in evapotranspiration was found over the FD regime. Only 38 mm (20.9%) and 55 mm (30.6%) of irrigation water went into the drainage, most of the supplementary irrigation was routed to the soil profile to maintain the water table.

3.3.2. Crop growth and yield

Except for an 8-day delay in simulated (vs. measured) crop maturity date in 2008, the RZWQM2 model simulated different crop growth stages within 0–3 days (Table 3.10). The simulated phenological dates in 2009 were also reasonable, with simulated emergence being 3 days late, silking date one day earlier and maturity date 3 days earlier. Accuracy statistics show a good model prediction of LAI under three different N application rates under both FD and CD-SI irrigation regimes (Table 3.8). The NSE for the six treatment combinations ranged from 0.76 to 0.96, with IoA close to 1 for all treatments and PBIAS within 15%. Fig. 3.7 shows that the simulated LAI closely followed the observed LAI.

In both years simulated yield under FD was simulated exceptionally well (PBIAS $\approx$ 0%), while under CD-SI it was only over-estimated by 3% in 2008 and 2% in 2009 (Table 10). The field experiment indicated similar high yield (around 12 Mg ha^{-1}) for all the N application rate treatment under both FD system and CD-SI system in 2008. This lack of difference among treatments was perhaps the result of a more fertilizer-rich soil in 2008 (initial N application of 43 kg ha^{-1}) compared to 2009 (27 kg ha^{-1}) (Table 3.1). In the experimental field, peas (*Pisum sativum L.*) were planted in 2007, instead of corn, resulting in a better soil structure in the subsequent year (Singh, 2013). To simulate high yield, reasonable rates of mineralization and denitrification of initial N levels were set during calibration. The model output suggests that no nitrogen or water stress occurred under any of the treatments in 2008. However, in 2009 the simulated yield differed for both FD and CD-SI drainage management routines and under the different N applications rates as a result of N stress brought on by lower N applications.

3.4 Discussion

Opposite to the results reported by Stampfli and Madramootoo (2006) and Tan et al. (1997), both our measured data and the modeling results showed a lower yield under CD-SI than FD (Table 10). This concurs with observations at the same experimental site in 1998 and 1999, when yields were 25% and 1.7% greater under FD than CD-SI (Madramootoo et al., 2001). The crops subjected to the CD-SI drainage management scenario likely suffered from waterlogging when too much precipitation and irrigation were applied, causing the water table to rise to very high levels (Madramootoo et al., 2001). In our experiment, the average water table reached up to 20 cm below the surface, while in some plots even to the soil surface in early June and late July in the year of 2008. Similar results were also found in the thesis of Lu (2015), who simulated slightly lower corn and soybean yield under CD-SI than FD in 2008, 2009 and 2011 in Harrow, Ontario using RZWQM2. Meanwhile, there was no significant difference of the measured corn and soybean yield between FD and CD-SI, which was explained by sufficient rainfall for the crops in this area.

The present simulations showed no water stress to have occurred during the growing seasons; accordingly, no significance difference of crop yield was apparent between FD and CD-SI irrigation management scenarios in 2008, when no N stress occurred. However, in 2009 the crop under CD-SI sustained much more N stress than that under FD, which is consistent with the greater NO_3^- loss under the CD-SI (vs. FD) system, due to more drainage. Simulated growing season NO_3^- leaching under the CD-SI system was 39% and 34% greater than under the FD system in 2008 and 2009, respectively. The crop yield under different N applications were similar in 2008 due to the high initial N fertilization, but the greater N stress and excessive water under CD-SI in 2009 might account for the lower yields under CD-SI than FD. Our simulated N losses under CD-SI and FD showed adverse results compared to the experiments of Tan et al. (1997), who indicated 24% less NO_3^- - N losses under CD-SI system. This was because we opened the drains several times during the crop growing season when the water table reached to the ground, while they kept the drains closed for the whole growing season except planting and harvesting. Due to higher water supply from irrigation in our experiment, more water was drained from CD-SI and more N might be lost from drainage as a consequence.

Overall, lower crop yield under CD-SI could be attributed to higher N losses when drains were opened shortly after irrigation was implemented, or waterlogging when too much water was supplied to the soil profile. As RZWQM2 is not capable of simulating waterlogging effects, the model should be improved by adding a waterlogging subroutine to better predict crop growth under adverse conditions.

The RZWQM2 over-estimated the drainage in March and May. The Kalman Filter Algorithm significantly improved the accuracy of RZWQM2 simulated drainage by eliminating the errors. These errors might be attributable to the loss of snow cover through sublimation, which the model does not take into account. Moreover, water infiltration during spring freeze-thaw cycles may not be well simulated. In the fine sandy soil, the actual k_{sat} could be very low when the soil temperature was below 0 °C when most water was frozen (Burt and Williams, 1976), allowing little water flow through the soil. However, the model's calculations yield a winter period k_{sat} which differs little (2% lower) with the calibrated k_{sat} (Table 2), which ranged from 30 to 60 mm h^{-1} in the upper soil layers. To achieve a better understanding of winter soil hydraulics, soil temperatures, surface temperature and snow depth should be measured, thereby allowing a further evaluation of the model's capacity to simulate winter and early spring drainage. The drainage during the summer season in 2008 was under-estimated, which could be resulted from the over-estimation of ET. The RZWQM2 simulated annual ET were 612 and 528 mm for 2008 and 2009, the value of 2008 was much higher than the DRAIN-WARMF-simulated values by Dayyani et al. (2010a, b) for the same region from 1993 to 1996 (531 mm $\leqslant$ ET $\leqslant$ 566 mm). Since the sap flow was only measured on 35 days each year, a longer period of measurement is suggested for further model evaluation.

3.5 Summary and conclusions

The RZWQM2 model was calibrated and validated against a comprehensive dataset of measured subsurface drainage flow, water table depth, soil water content, crop transpiration, leaf area index, yield, and phenological crop development stages for corn grown in a subsurface drained field in Southern Quebec. Given the challenges in fitting predicted results with such a comprehensive measured dataset, the RZWQM2 model performed well in simulating the hydrologic cycle and corn growth. Soil water content was simulated within an acceptable range in terms of PBIAS. Nevertheless, the model performed well in simulating the crop growth stage, yield and LAI under different N application rates and drainage modes. The calibration and validation phase overestimation of drainage flow in winter and spring was minimized using a variant RZWQM2 model equipped with a Kalman filter algorithm. The resulting simulated values show a good correlation with the observed data; however, the Kalman filter is subject to the limitation that it works very well when the system error fits a Gaussian distribution, but for other systematic errors, it performs poorly. Although Kalman filter is a good approach to calibrate an imperfect winter drainage component, a better model calibration method is still needed. In addition, the linear Kalman filter algorithm used in this paper is not applicable for reducing the nonlinear errors within the model. These errors can be caused by human activities or other unknown environmental factors. In the recent years, the artificial neural network has showed excellent performance in nonlinear model estimation, therefore, future work would be (i) try the artificial neural network which better describes the nonlinear system to improve the model prediction (ii) measure sap flow for a longer period or measure the ET across the full year to get more reliable observed data for model calibration.

Acknowledgements

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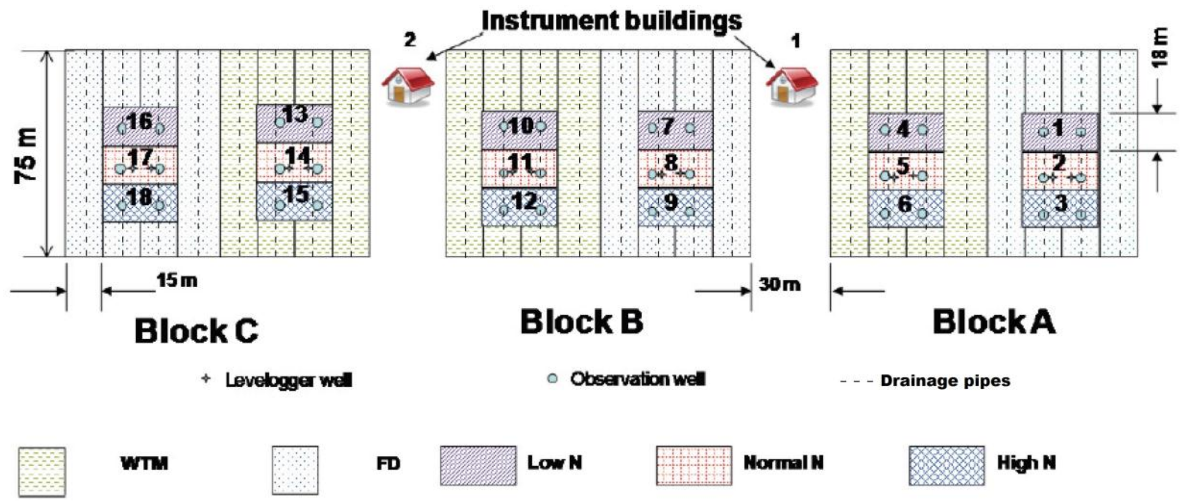

Figure 3.1. Experimental layout of field study (adopted from Singh et al. (2014)), WTM is the water table management of controlled drainage with subirrigation; FD is the free drainage

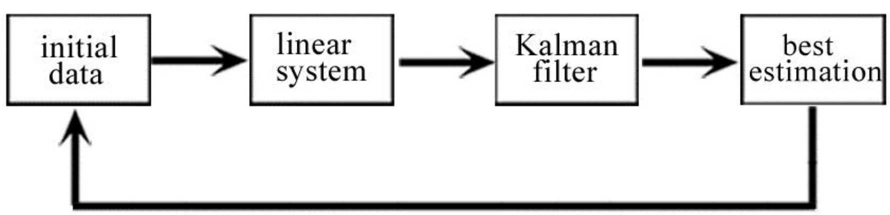

Figure 3.2. The process of Kalman filter in this study

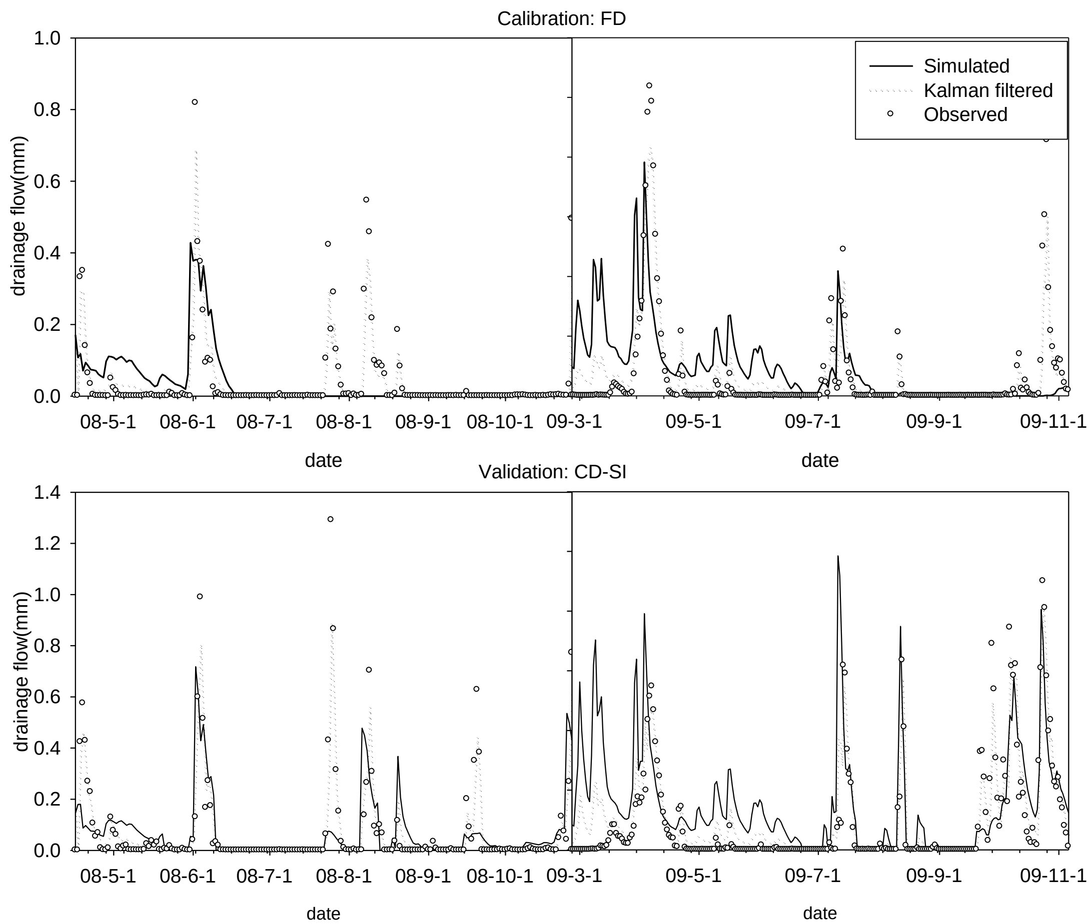

Figure 3.3. Comparison of observed drainage, RZWQM2-simulated drainage, and Kalman-filtered drainage.

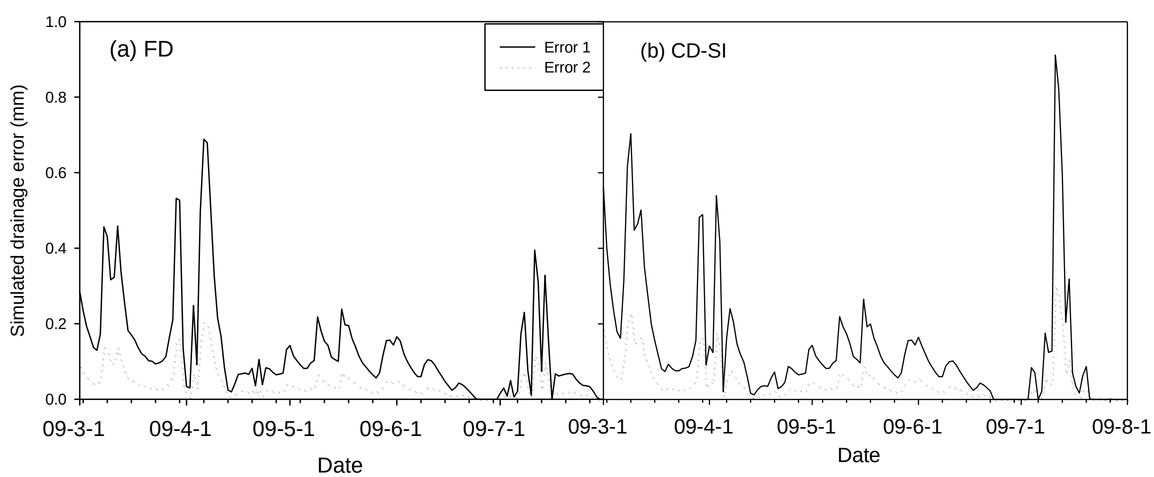

Figure 3.4. The comparison of errors between simulated and observed results: RZWQM2 error (error 1) and RZWQM2-Kalman error (error 2) under FD (a) and CD-SI (b)

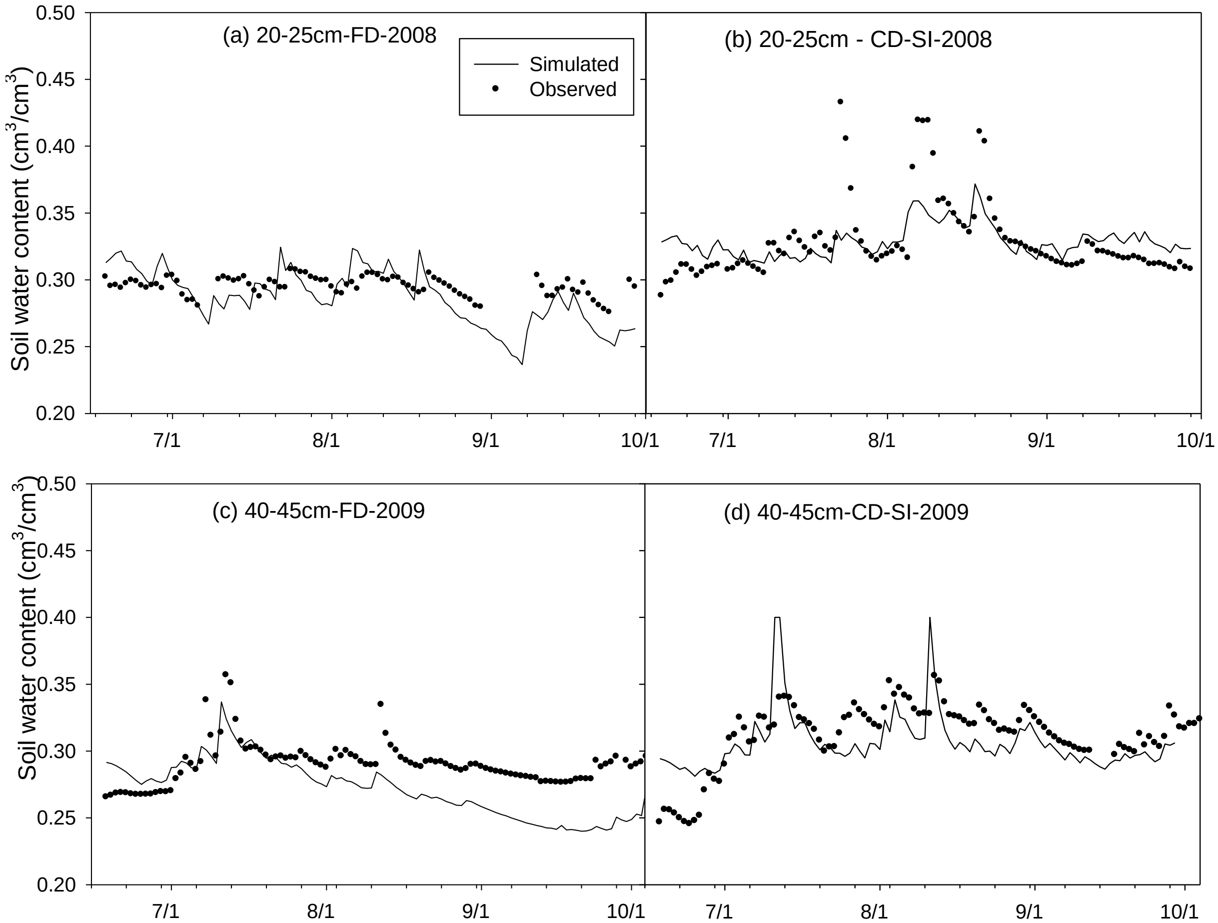

Figure 3.5. Simulated and observed daily soil water content (0.20-0.25 m depth in 2008, 0.40-0.45 m depth in 2009) for free drainage - FD (a, c) and controlled drainage with sub-irrigation – CD-SI (b, d)

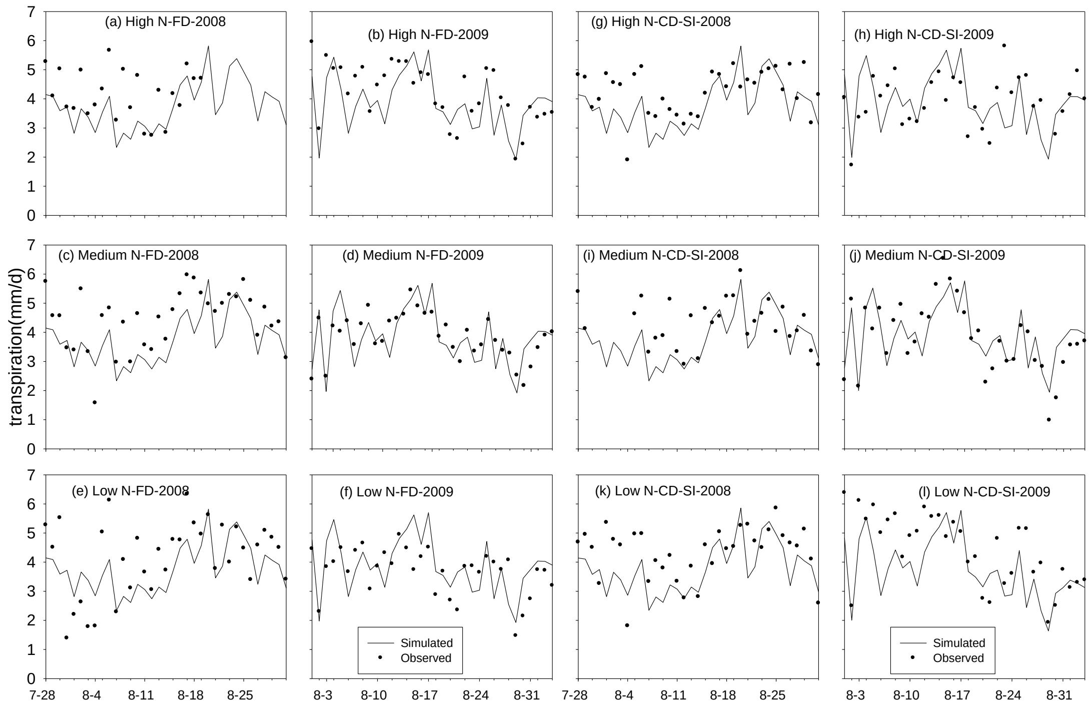

Figure 3.6. Simulated daily transpiration and observed sap flow under FD (a-f) and CD-SI (g-l)

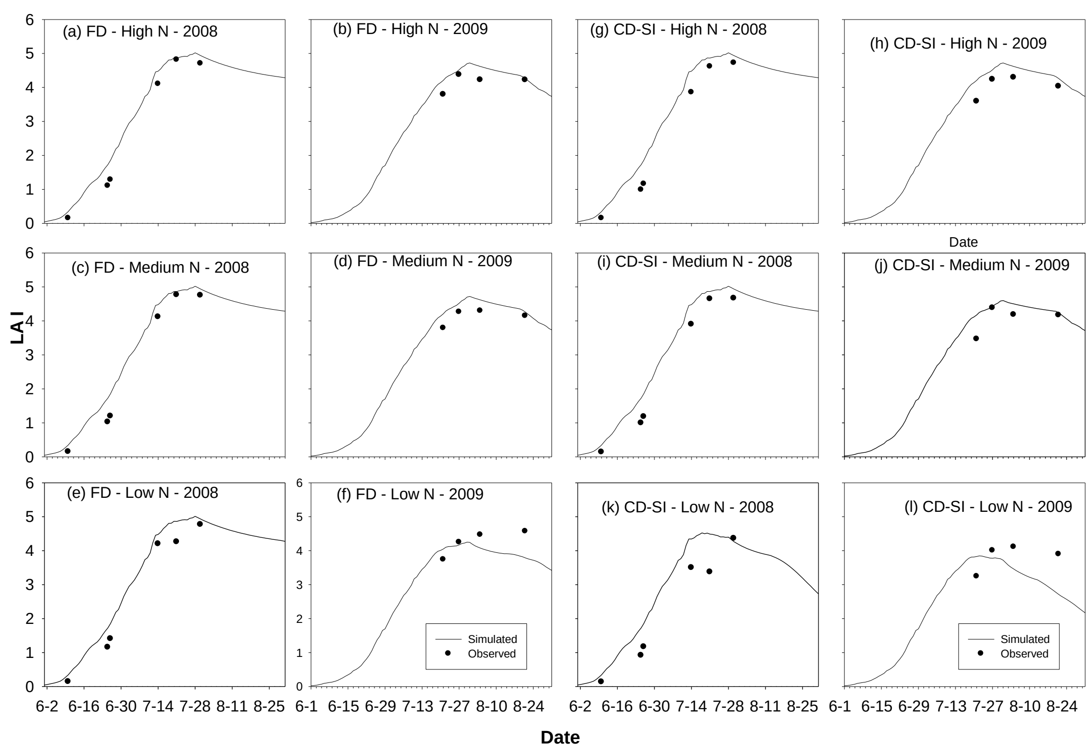

Figure 3.7. Simulated and observed LAI under FD (a-f) and CD-SI (g-l), under three nitrogen fertilization regimes, across two years (2008, 2009)

Table 3.1. N application rate and soil residual N before planting (Unit kg N ha^{-1})

N application	2008				2009			
	Date	**Low N**	**Medium N**	**High N**	**Date**	**Low N**	**Medium N**	**High N**
1st	2-May	88	88	88	2-May	52	52	52
2nd	5-May	0	24	24	8-Jun	33	100	167
3rd	17-Jun	0	30	122	-	-	-	-
Initial N*		43	43	43		27	27	27
Total N		**131**	**186**	**277**		**112**	**179**	**246**

*Initial inorganic residual N before planting.

Table 3.2. Calibrated parameters for soil hydraulic properties.

Layer	Depth (m)	ρ (Mg m^{-3})	Soil Water Retention θ_s (m^3m^{-3})	θ_r (m^3m^{-3})	τb (mm)	λ	Lateral k_{sat} (mm h^{-1})	Vertical k_{sat} (mm h^{-1})	SRGF
1	0-0.15	1.4	0.452	0.075	-100	0.234	50	30	1.0
2	0.15-0.35	1.5	0.424	0.071	-180	0.224	50	30	1.0
3	0.35-0.45	1.4	0.400	0.041	-100	0.232	50	30	0.30
4	0.45-0.80	1.3	0.460	0.075	-156	0.320	120	60	0.07
5	0.80-1.20	1.4	0.464	0.075	-156	0.304	20	10	0.07
6	1.20-1.70	1.4	0.464	0.075	-156	0.304	20	10	0.01
7	1.70-2.30	1.4	0.464	0.075	-156	0.304	20	10	0.01
8	2.30-3.00	1.4	0.464	0.075	-156	0.304	20	10	0.01
9	3.00-3.80	1.4	0.464	0.075	-156	0.304	20	10	0.01
10	3.80-3.97	1.4	0.464	0.075	-156	0.304	20	0.1	0.01

[a] ρ = bulk density, θ_s = saturated soil water content, θ_r = residual soil water content, τb = bubbling pressure, λ = pore size distribution index, k_{sat} =saturated hydraulic conductivity; SRGF = soil root growth factor.

[b] Other required parameters include A1 (set to zero), B (computed using the RZWQM default constraint) for all layers, N_1 (set to zero), and K_2 and N_2 (computed using the RZWQM default constraints) for all layers (Ahuja et al., 2000b). The lateral hydraulic gradient was adjusted to a value of 1.5×10^{-6}.

Table 3.3. Calibrated parameters in RZWQM2 model.

Non-default Parameters	Value
Hydrology component	
Minimum leaf stomatal resistance (s m^{-1})	150
Albedo of dry soil	0.2
Albedo of wet soil	0.3
Albedo of crop	0.3
Albedo of fresh residue	0.3
Drain depth (m)	1.00
Drain spacing (m)	15.0
Radius of drain (m)	7.6
Surface soil resistance for S-W	250
Nutrient component	
Slow residue pool to intermediate soil	0.3
Fast residue pool to Fast soil humus pool	0.6
Fast soil humus pool to intermediate soil	0.6
Intermediate soil to slow soil humus pool	0.4
Concentration of NO_3^- in rainwater (mg L^{-1})	1.2
Aerobic heterotrophs	4×10^{-37}
Anaerobic	5×10^{-33}

Table 3.4. Calibrated crop parameters for maize (adapted from Ma, et al. 2011)

Calibrated Parameters	Value	Range
P1 Degree days (base temperature of 8 ℃) from seedling emergence to end of juvenile phase.	200	100-450
P2 Day length sensitivity coefficient [the extent (days) that development is delayed for each hour increase in photoperiod above the longest photoperiod (12.5 h) at which development proceeds at maximum rate].	0.3	0-2
P5 Degree days (base temperature of 8 ℃) from silking to physiological maturity	610	600-1000
G2 Maximum possible number of kernels per plant	950	400-1000
G3 Kernel filling rate during linear grain filling stage under optimum conditions(g/d)	14.5	5-16
PHINT Phylochron interval between successive leaf tip appearance	36	36-55
Maximum plant height at maturity (cm)	200	-
Plant biomass at half of maximum height (g)	18	-

Table 3.5. RZWQM2 and Kalman-modified RZWQM2 model accuracy statistics for daily drainage for FD (calibration) and CD-SI (validation) in 2008 and 2009 (unit: cm)

Model Accuracy Statistics	**FD**			**CD-SI**		
	Observed	RZWQM2	Kalman-RZWQM2	Observed	RZWQM2	Kalman-RZWQM2
Mean	0.05	0.07	0.05	0.08	0.12	0.09
Total	22.58	29.36	24.59	36.69	52.6	42.08
PBIAS		30%	9%		43%	15%
NSE		-0.01	0.91		-0.02	0.89
IoA		0.60	0.97		0.66	0.97

Table 3.6. Simulated and observed monthly drainage rate and accuracy statistics for RZWQM2 and Kalman-modified RZWQM2 models for FD and CD-SI drainage regimes implemented in 2008 and 2009, from April to October (monthly data not available for April in 2008 (unit: mm))

Year	Month	FD			CD-SI		
		Obs	RZWQM2	Kalman-RZWQM2	Obs	RZWQM2	Kalman-RZWQM2
2008	**May**	0.7	22.7	7.0	3.5	15.8	7.3
	Jun	23.6	32.3	26.1	29.5	34.6	31.2
	Jul	12.6	0	8.9	31.6	3.8	22.5
	Aug	22.5	0	15.7	19.1	32.2	23.4
	Sept	0.1	0	0.1	17.4	6.4	13.8
	Oct	5.6	7.4	6	13.7	27.9	18.5
2009	**April**	76.5	55.7	70.2	45.9	56.1	49.3
	May	2.2	41.1	13.8	1.6	41.2	14.7
	Jun	0.1	16.3	4.9	0.3	16.2	5.6
	Jul	23.9	26.9	24.7	23.9	48.5	32
	Aug	3.8	0.1	2.7	14.3	24.3	17.6
	Sept	0	0	0	29.0	8.3	22.2
	Oct	33.4	0.2	24.1	94.9	91.5	95.9
Accuracy Statistics	**Sum**	**205.0**	**202.7**	**204.1**	**325**	**406.8**	**354.1**
	Mean	**15.8**	**15.6**	**15.7**	**25**	**31.3**	**27.2**
	PBIAS		**-1.1%**	**-0.4%**		**25.2%**	**9.0%**
	NSE		**0.18**	**0.93**		**0.39**	**0.93**
	IoA		**0.75**	**0.98**		**0.83**	**0.98**

Table 3.7. RZWQM2 performance statistics for soil water content simulations.

Model Accuracy Statistic	Drainage regime Soil depth (year)			
	FD		CD-SI	
	0.20-0.25 m (2008)	0.40-0.45 m (2009)	0.20-0.25 m (2008)	0.40-0.45 m (2009)
RMSE (cm^3/cm^3)	0.05	0.04	0.03	0.04
RRMSE	17.9%	12.0%	8.7%	10.6%
PBIAS	6%	0%	-1%	0%
NSE	0.05	0.18	-1.78	-0.02
IoA	0.27	0.39	0.47	0.73

Table 3.8. RZWQM2 performance statistics of simulated daily transpiration *vs.* measured sap flow and leaf area index (LAI). ET is the evapotranspiration (unit: mm).

	Model Accuracy Statistics	FD			CD-SI		
		High N	Medium N	Low N	High N	Medium N	Low N
transpiration	**NSE**	0	0.32	0.24	0	0.37	0.03
	RMSE (mm)	0.82	0.81	0.98	0.97	0.75	1.03
	RRMSE	20%	21%	27%	24%	19%	23%
	PBIAS	8%	0%	-6%	6%	2%	14%
	IoA	0.71	0.78	0.72	0.69	0.69	0.68
	ET-2008	612	612	611	601	601	606
	ET-2009	574	574	584	531	528	530
LAI	**NSE**	0.96	0.95	0.93	0.92	0.92	0.76
	PBIAS	9%	10%	4%	13%	-12%	-9%
	RMSE	0.363	0.39	0.44	0.484	0.46	0.71
	RRMSE	11%	12%	13%	15%	14%	25%
	IoA	0.99	0.99	0.98	0.91	0.91	0.93

Table 3.9. Soil water balance for FD and CD-SI drainage management regimes during the growing seasons (May-Sept) of 2008 and 2009 (unit: mm).

Drainage regime - Year	Water Balance (mm)					
	Inputs (S)		Withdrawals (W)			ΔS-W
	precipitation	irrigation	E_a	T_a	drainage	
FD 08	432	0	150	402	55	-174
FD 09	462	0	134	368	84	-123
CD-SI 08	432	182	146	403	93	-27
CD-SI 09	462	180	134	367	139	-3

Note: E_a, T_a, ΔS-W, are actual evaporation, actual transpiration, and change in soil water storage, respectively.

Table 3.10. Simulated (sim) and observed (obs) crop growth stages across all drainage × N fertilization treatments, and model accuracy statistics for crop yield (unit: Mg ha^{-1}) under different treatments. Planting occurred on May 4 and May 7 in 2008 and 2009, respectively.

Phenological stage	Year of Growing Season					
	2008			2009		
	obs	sim	Difference	obs	sim	Difference
Emergence	May 16	May 18	+2	May 19	May 22	+3
Silking	July 30	July 29	-1	Aug 2	Aug 1	-1
Maturity	Sept 21	Sept 29	+8	Sept 24	Sept 25	+1

Nitrogen level	FD		CD-SI		FD		CD-SI	
	obs	sim	obs	sim	obs	sim	obs	sim
Corn yield (Mg ha^{-1})								
Low N	12.46	12.4	12.38	9.17	10.75	10.55	8.80	7.35
Medium N	12.59	12.58	11.97	11.03	11.20	11.71	10.87	9.12
High N	12.58	12.58	12.37	12.58	12.14	11.78	11.55	10.66
Mean	12.54	12.52	12.24	10.93	11.37	11.35	10.41	9.04
Model Accuracy Statistics								
RMSE	0.03		1.93		0.36		1.41	
RRMSE	0%		16%		3%		14%	
PBIAS	0%		-11%		0%		-13%	

Connecting text to Chapter 4

Chapter 3 comprehensively evaluated the RZWQM2 in simulating the hydraulic and crop growth components using a full dataset, which provided a sound basis for the simulation of nutrient movement in soil and water in subsurface-drained fields. Chapter 4 tested the RZWQM2 and comparted its ability with a widely used C: N cycling model, DNDC. The two models' performances in predicting soil temperature, soil water content, N_2O and CO_2 emissions, corn and soybean yields, as well as daily drainage in growing seasons were compared, meanwhile advantages and disadvantages of each model were discussed. The following manuscript, co-authored by Dr. Zhiming Qi, Chandra A. Madramootoo, Ward Smith, Naeem A. Abbasi, Tie-Quan Zhang has been submitted to Geoderma.

Jiang, Q., Qi, Z., Madramootoo, C.A., Smith, W., Zhang, Abbasi, N.A., Zhang, T.Q., 2018. Comparison of RZWQM2 and DNDC model in simulating greenhouse gas emissions, crop yield and subsurface drainage. Geoderma (submitted).

Chapter 4

Comparison of RZWQM2 and DNDC model in simulating greenhouse gas emission, crop yield and subsurface drainage

Qianjing Jiang, Zhiming Qi, Chandra A. Madramootoo, Ward Smith, Naeem A. Abbasi, Tie-Quan Zhang

Abstract

Process-based models are promising tools for developing management practices that may mitigate greenhouse gas emissions. In this study, the newly developed greenhouse gas emission component and sub-irrigation module of the Root Zone Water Quality Model (RZWQM2) were tested and subsequently compared with the DNDC (DeNitrification–DeComposition) model using measured data from a subsurface drained and irrigated field with corn-soybean rotation in Southern Ontario, Canada. Field measured data included N_2O and CO_2 flux, soil temperature, soil moisture content, tile drainage and crop yield from a four-year field experiment (2012 - 2015). The experiment was composed of four treatments: tile drainage and inorganic fertilizer (DR-IF), controlled drainage with subirrigation and inorganic fertilizer (CDS-IF), tile drainage and solid cattle manure (DR-SCM), controlled drainage with sub-irrigation and solid cattle manure (CDS-SCM). Both models were calibrated using the data from DR-IF. RZWQM2 was validated using all three remaining treatments while DNDC was validated only for DR-SCM since it does not characterize controlled drainage and sub-irrigation. Statistical results indicated that DNDC had better ability in simulating soil temperature than RZWQM2, but RZWQM2 performed better than DNDC in simulating soil water content (SWC) due to the lack of a heterogeneous soil profile, shallow simulation depth and lack of crop root density functions. RZWQM2 predicted the cumulative N_2O emission and CO_2 emission within 15% error under all four treatments. DNDC performed similarly under the two treatments, except the timing of CO_2

emissions was better predicted by RZWQM2 (RMSE = 0.43-0.59) than by DNDC (RMSE = 0.62-0.79). Both models accurately estimated cumulative drainage within 15% error during the growing season, but RZWQM2 was more accurate in predicting the daily drainage under different water table management. Both models performed satisfactorily in predicting grain yields of corn and soybean with PBIAS within 15%. Overall, RZWQM2 required more experienced and intensive calibration and validation, but it provided more accurate predictions of soil hydrology and better timing of CO_2 emissions than did DNDC.

Key words: controlled drainage; subirrigation; water table management; manure application; inorganic fertilization; corn-soybean rotation

4.1 Introduction

Agricultural activities directly contribute 20% of the total global greenhouse gas (GHG) emissions (Lokupitiya and Paustian, 2006). In Canada, 18.5% of national CO_2, 28% of CH_4, and 71% of N_2O gases are produced from agriculture activities (ECCC, 2017). N_2O is mainly emitted from the nitrification and denitrification process in the soil profile, while the major source of CO_2 production is from residue decomposition and aerobic respiration of microorganisms and roots. Greenhouse gas emissions are affected by soil type, soil pH, soil temperature, soil moisture content, soil oxygen content, and nutrient availability (Oertel et al., 2016). Agricultural management practices play an important role in the production of GHG, such as fertilization, manure application, tillage, cover crops, incorporation of crop residue, drainage and irrigation. It is reported that 22% of the total agricultural GHG emissions in Canada are attributed to the application of inorganic fertilization (ECCC, 2017). Drainage helps to improve crop productivity and increases soil organic carbon (SOC) through higher crop C inputs in humid areas and has the potential to reduce N_2O emission from agricultural soils by promoting aerobic conditions, however, it may also result in higher N losses through tile drains (Smith et al., 2008a).

Chambers techniques are widely employed for measuring site specific GHG emissions, however it can be difficult to extrapolate these observations over larger scales since the values are highly relevant to the specific soil properties, weather conditions and agronomic activities (Smith et al., 2002). Micrometeorological techniques for measuring N_2O emissions at a plot and field scale are costly, laborious and time intensive thus there are only a few locations in Canada where these techniques are used. As a consequence, there have been efforts to develop and validate biophysical models for simulating GHG emissions temporally and spatially under diverse cropping systems and evaluating the impacts of beneficial management practices (Brilli et al., 2017). Process-based models have been developed and tested for estimating GHG emissions, such as DAYCENT (Parton et al. 1998), DNDC (Li et al., 1992) and WNMM (Li et al., 2007). These models enrich people's understanding of the complicated physical, microbial and chemical processes in the soil profile through comparison with the observations, and provide estimates of soil responses to climate change and some other conditions (Necpálová et al., 2015). The DNDC (Denitrification–Decomposition) model includes algorithms for simulating N_2O, CO_2, CH_4, N_2 and NO_x fluxes from cropping systems, livestock and farm facilities (Li et al., 2012) and was found to be the only model capable of simulating all trace gas fluxes considered in an asessment of 9 prominent GHG models (Brill et al., 2017). The model has been improved and evaluated for simulating N_2O emission prediction in Canada (Smith et al., 2002; Smith et al., 2008b; Smith et al., 2013; Abalos et al., 2016; He et al., 2018), India (Pathak et al., 2005), China (Cai et al., 2003; Zhang et al., 2015), New Zealand (Saggar et al., 2007), Europe (Levy et al., 2007), and globally (Ehrhardt et al., 2018). Evaluations have also been extended to methane production (Badu et al., 2006; Fumoto et al.,2008), NH_3 volatilization (Congreves et al., 2015; Dutta et al., 2016), net CO_2 emissions (Yadav and Wang, 2017; Li et al., 2017) and SOC (Wang et al., 2008; Qiu et al., 2005; Smith et al., 2012; Grant et al., 2016; Dutta et al., 2017). Yadav and Wang (2017) modified the DNDC model to simulate CO_2 emission from three agricultural sites in Saskatchewan, Canada. The model estimated annual CO_2 emissions reasonably in comparison to observations and predicted that CO_2 emissions decreased when reducing the amount of fertilizer and irrigation.

Although process-based models are promising tools for estimating GHG emissions, uncertainties still exist due to the complex nature of agroecosystems and our limited understanding of biogeochemical processes (Brilli et al., 2017; Ehrhardt et al., 2018). For example, DNDC was reported to correctly predict the seasonal N_2O emission but failed to capture the peaks of daily N_2O flux (Babu et al., 2006) or simulate the timing of N_2O peaks (Smith et al., 2002; Smith et al. 2008b). Beheydt et al. (2007) found that DNDC predicted higher and more frequent N_2O peaks compared to field measurements. Smith at al. (2008b) compared the performance of DNDC and DAYCENT model in simulating N_2O emission in Quebec and Woodslee under different N fertilization and tillage practices. The DNDC model performed better than DAYCENT in simulating the seasonal N_2O emissions, while both models had difficulties in simulating the daily N_2O flux. The performance of DNDC has also been compared by Wu and Zhang (2014) to the WNMM and DAYCENT models and was judged as the best one for predicting the daily N_2O emission and continuous seasonal emission, while Li et al. (2005) stated that WNMM performed better than DNDC and DAYCENT since the latter two models over-estimated the temporal N_2O by 40%. In a global study using 24 models (including DNDCv.CAN and DayCent) with simulations across 10 experimental sites it was found that the model ensemble produced an RMSE of less than 60% for N_2O emissions for wheat, corn and rice (Ehrhardt et al., 2018). DNDCv.CAN was chosen as one of the 3 models for annual cropping, to be used in a reduced model ensemble.

The model accuracy of N_2O emission prediction is highly dependent on the accurate estimation of soil water content, soil temperature, and the concentration of NH_4^+ and NO_3^- in the top layer of the soil profile (Li et al., 2004). RZWQM2 is a comprehensive one-dimensional model which can be used to study the interaction of physical, chemical, and biological processes within the soil profile (Ahuja et al., 2000). It has been extensively tested for simulating hydrology (Singh et al., 1996, Akhand et al., 2003, Abrahamson et al., 2006), N dynamics (Cameira et al., 2007, Qi et al., 2011, Qi et al., 2012), crop production (Ma et al., 2007, Saseendran et al., 2007, Thorp et al., 2007), and pesticides transport (Bakhsh et al., 2004, Malone et al., 2014). Fang et al. (2015) improved RZWQM2 by incorporating the algorithm for computing N_2O emission from nitrification based on the NOE model and N_2O emission from the denitrification algorithm in the DAYCENT model to predict N_2O emission from the soil profile. Gillette et al. (2017) tested the modified RZWQM2 model in predicting the effect of tillage and N fertilization amount on N_2O emissions in an irrigated corn field in Colorado, indicating that it slightly underestimated N_2O emissions by 1.5% and 7.1% under no-tillage and conventional tillage. Jiang et al. (2017) evaluated RZWQM2 for predicting N_2O and CO_2 emission in a subsurface drained field in Southern Quebec under water table management, and used the calibrated model to investigate different agronomic management impacts on GHG emissions. However, the modified RZWQM2 model has not been tested for predicting emissions under manure application, nor has it been compared to other C/N models to verify its ability in predicting GHG emissions. The objectives of this study are to 1) evaluate the GHG emission and subirrigation components of RZWQM2 under different water table management practices, inorganic fertilizer and organic manure application; 2) compare the performance of RZWQM2 with DNDC, a widely used C/N cycling model, for simulating GHG emissions, crop yield and drainage flow in a subsurface drained and irrigated field under soybean-corn rotation.

4.2 Methods and materials

4.2.1 Field experiment

The field study was conducted from 2012 to 2015 at the Hon. Eugene F. Whelan Research Farm, near South Woodslee, Ontario, Canada (42°13′ N, 82°44′ W). Experimental plots were equipped with subsurface drainage and sub-irrigation with a corn-soybean rotation cropping system. The soil type was Brookston clay loam with average soil bulk density of 1.46 g cm^{-3} and a porosity of 44.9%. The faction of clay, sand and silt was 37%, 28% and 35%, respectively. The saturated hydraulic conductivity ranged from 0.07 to 0.50 cm per hour (Lu, 2015). The annual precipitation was 643, 998, 800, 843 mm in the years of 2012, 2013, 2014 and 2015, respectively. The weather data, including daily precipitation, relative humidity, minimum temperature, maximum temperature, and wind speed were measured at the experimental site. The field slope was 0.5% on average.

Each of the four treatments were assigned to two plots but the GHG data was only collected in one plot with 6 replicate chambers: 1) plot 9, tile drainage and inorganic fertilization (DR-IF); 2) plot 10, controlled drainage with sub-irrigation and inorganic fertilization (CDS-IF); 3) plot 12, tile drainage and solid cattle manure (DR-SCM); 4) plot 13, controlled drainage with sub-irrigation and solid cattle manure (CDS-SCM). A corn-soybean rotation system was used with corn (Syngenta NK N459-3000GT) grown in 2012 and 2014 while soybean (Pioneer 92Y53) was grown in 2013 and 2015. The N fertilization was applied only in 2012 and 2014 before corn planting (Table 1). The tile drains were installed at the soil depth of 0.85 m. For the CDS system the water table was constantly controlled at 46 cm and during the sub-irrigation period (from June 22nd to August 8th in 2012) the head gate was maintained at 20 cm. The tile drainage volume was collected in the instrumentation building using tipping buckets. Each tipping bucket was connected to a data logger and the tipping rates were used to calculate drainage volume.

Soil temperature (0–10 cm) was measured in situ using the TidbiT devices (HOBO TidbiT v2 Water Temperature Data Logger) at the same times and locations as the GHG measurements, and volumetric soil water content was measured (0–10 cm) using the HH2 moisture meter with Theta probe type ML2x (Delta-T Devices, Cambridge, England). The N_2O and CO_2 flux was collected weekly during the growing season from 2012 to 2015 using six closed Plexiglas chambers (0.556 m $\times$ 0.556 m $\times$ 0.140 m) in each plot. The chambers were inserted 10 cm deep into the soil profile, and on top of each chamber a vent tube port was used to prevent air exchange. The GHG measurements in each chamber were taken five times at 15 minute intervals, and averaged from six chambers for each plot.

4.2.2 Model description

4.2.2.1 Overview of RZWQM

The RZWQM is a one-dimensional process-based model that integrates the physical, chemical, and biological processes within the soil profile to simulate plant growth, movement of water and chemicals in water (Ahuja et al., 2000). The Green-Ampt equation (Green and Ampt, 1911) is used for computing water infiltration after precipitation and irrigation events, then the Richards equation is used for redistributing water in the soil profile (Richards, 1931). The drainage flux is calculated using the Hooghoudt equation (Bouwer and Van Schilfgaarde, 1963) and potential evapotranspiration is described by the Shuttleworth-Wallace equation

(Shuttleworth and Wallace, 1985). Sub-irrigation is applied to a user-defined depth in the soil profile and redistributed using the Richards equation.

The RZWQM2 computes the nitrification and denitrification rates using zero and first-order kinetics (Ahuja et al., 2000), as functions of NH_4^+ concentration, NO_3^- concentration, soil temperature, soil water and a series of constants. Fang et al. (2015) incorporated the algorithms for computing the N_2O emissions from nitrification and denitrification from NOE and the DAYCENT models, respectively, after comparing four C: N cycling models. The detailed equations of nitrification and denitrification rates, N_2O and CO_2 emissions are presented in section 2.3.2 in this thesis.

4.2.2.2 Overview of DNDC

The DNDC model was initially developed by Li at al. (1992) for simulating N_2O emissions from agricultural soils, and numerical modifications have been made to expand its applicability to estimate CO_2 emissions and soil C and N cycling (Li et al., 1994), water and N movement through the soil profile and loss to tile drains (Li et al., 1996), and CH_4 and NH_3 emissions from cropping systems, livestock and full farm facilities (Li et al., 2012). DNDC consists of four sub-models, including the soil climate sub-model, plant growth sub-model, denitrification sub-model, and decomposition sub-model (Li et al., 1994).

Recently, a regional version of DNDC was developed (DNDCv.CAN) which includes improved crop growth with better simulation of the impacts of temperature, water and nutrient stress for cool season cultivars in Canada (Kröbel et al., 2011; Smith et al., 2013; Grant et al., 2016). Smith et al. (2013) improved the response of elevated atmospheric CO_2 concentration on crop water and nitrogen use efficiency and Dutta et al. (2016) revised the ET routine to include

FAO Penman–Monteith equations and crop coefficients (Dutta et al., 2016). Soil evaporation is affected by crop residue cover and soil moisture in the top 15 cm of the profile, while the plant transpiration is estimated from the crop water requirement which is determined by the crop biomass and the crop water use parameter specific to each crop type. Transpiration is limited by soil water availability and the rate of uptake by roots (Sansoulet, et al., 2014).

DNDC simulates N_2O emissions in response to nitrification and denitrification processes. The nitrification rate is computed as follows:

$$R_n = 0.005 \times [NH_4] \times Nitrifier \times f(pH) \qquad [4.1]$$

The N_2O emission from nitrification is computed as a function of the nitrification rate, WFPS and temperature factor:

$$N_2O_{nitri} = 0.0006 R_n F_t WFPS \qquad [4.2]$$

Where Nitrifier is the microbial biomass of nitrifiers (the growth and death rates are dependent on dissolved organic carbon and soil moisture content), $[NH_4]$ is the concentration of ammonium (kg N ha^{-1}) and pH is the soil pH value. F_t is the temperature factor for nitrification and WFPS is the water-filled pore space. The nitrifier biomass is computed using the relative growth and death rates of nitrifiers, soil moisture factor and soil temperature factor.

The process of denitrification in DNDC model is expressed as the reduction of NO_3^- to NO_2^-, NO and N_2O, and finally N_2 based on a series of environmental factors such as pH, soil organic carbon, microbial populations and temperature. The consumption of NO_x (NO_3^-, NO_2^-, NO and N_2O) is expressed as:

$$\frac{d(NO_x)}{dt} = \left(\frac{u_{NO_x}}{Y_{NO_x}} + M_{NO_x} \times \frac{[NO_x]}{[N]}\right) \times Denitrifier \times F_{pH-NO_x} \times F_T \qquad [4.3]$$

Where u_{NO_x} is the relative growth rate of NO_3^-, NO_2^-, NO and N_2O denitrifiers, Y_{NO_x} is the maximum growth yield on NO_3^-, NO_2^-, NO and N_2O, M_{NO_x} is the maintenance coefficient of NO_3^-, NO_2^-, NO and N_2O, $[N]$ is the total nitrogen as the sum of NO_3^-, NO_2^-, NO and N_2O, F_T is the temperature factor, F_{pH-NO_x} is the soil pH factor, and Denitrifier is the biomass of denitrifier bacteria.

In DNDC, N gas emissions are regulated by an "anaerobic balloon" concept where the Nernst equation is used to estimate redox potential (Eh) which regulates the size of the aerobic (nitrifier) and anaerobic (denitrifier) microbial fractions. The aerobic portion is considered to be outside the balloon and the anaerobic inside. The balloon will swell at lower Eh or higher so oxygen content. The Nernst equation thermodynamically determines if nitrification or denitrification occurs and further determines when specific biologically-mediated reductive reactions from $NO_3 \rightarrow NO_2 \rightarrow NO \rightarrow N_2O \rightarrow N_2$ occur. The redox potential is estimated as follows:

$$E_h = E_o + \frac{RT}{nF} \times \ln(\frac{OX}{RE}) \qquad [4.4]$$

Where Eh is the redox potential (volts), Eo 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^{-1}), respectively.

In the denitrificiation submodel, the quantity of denitrifier-bacteria is estimated using a multi-nutrient dependent (Michaelis–Menten) growth function dependent on temperature, DOC, soil water, Eh, and pH, kinetically determining the growth rate as follows:

$$R = R_{max} \times DOC/(\,K_a + DOC) \times OX/(K_b + OX) \qquad [4.5]$$

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 R_{max} were taken from a laboratory study by Leffelaar and Wessel (1998). The DNDC model computes the daily CO_2 emission from aerobic respiration of microbial organisms, crop roots, stem and leaves. Soil organic carbon (SOC) is used as the energy source to produce CO_2, and the rate is computed using the equation (UNH, 2017):

$$dC/dt = CNR \times \mu \times (S \times kl + (1 - S) \times kr) \times [C] \quad [4.6]$$

Where $[C]$ is the concentration of organic C (kg C ha^{-1}), t is time (day), S is labile fraction of organic matter in the pool, (1-S) is the resistant fraction of organic C compounds, kl and kr are the specific decomposition rates (SDR) of labile and resistant fractions, μ is the temperature and moisture factor, and CNR is the C/N ratio reduction factor. SDR is 0.074, 0.074, 0.02, 0.33, 0.04, 0.16 and 0.006 for very labile litter, labile litter, resistant litter, labile microbes, resistant microbes, labile humads, and resistant humads, respectively.

4.2.3 RZWQM2 model simulation

Meteorological data that was used for both models included maximum and minimum temperature, wind speed, relative humidity, solar radiation and precipitation. The hydrologic component was calibrated against the measured daily soil moisture and drainage data from plot 9 (DR-IF) and validated using measured data from plot 10 (DR-SCM), plot 12 (CDS-IF) and plot 13 (CDS-SCM). The drainage flux was not simulated under DR-SCM due to the unavailability of measured data. The calibrated soil hydraulic parameters are listed in Table 4.2. The nutrient parameters were calibrated to match the GHG measurement. The interpool transformation coefficient for the slow residue pool to intermediate soil humus pool was adjusted from a default value 0.1 to 0.3, and the fast residue pool to fast soil humus pool transformation coefficient was increased from 0.1 to 0.6. The denitrification rate was reduced from 1.0×10^{-13} to 2.0×10^{-14} (Table 4.3). The model was run for 10 years prior to the simulation period to properly initialize the soil microbial populations as suggested by Ma et al. (1998).

4.2.4 DNDC model simulation

In this study, the Canadian regional version of DNDC, DNDCv.CAN was applied to simulate GHG emissions, crop production and drainage. Soil parameters were calibrated or set based on measurements (Table 4.4). The DNDC model was run for 10 years (from 2002 to 2011) prior to the simulation to stabilize soil N and C. Since the DNDC model does not include a sub-irrigation component, it was calibrated using observed data of soil moisture, soil temperature, GHG flux, crop yield and drainage under DR-IF and validated only using the DR-SCM treatment. DNDC did not include algorithms for mechanistic tile drainage, thus the total water leached below 100 cm was considered the water loss to the drains. To obtain reasonable drainage, the soil parameters in Table 4.4 were calibrated, and evapotranspiration was adjusted by changing the crop water demand.

For both corn and soybean, the physiological and phenological parameters were adjusted to calibrate crop yield, and biomass fractions were also adjusted to improve CO_2 simulation. Default values were kept for the other crop parameters. The nutrient parameters available to users are limited, including: initial soil nitrate and ammonium, microbial activity parameters, soil organic matter partitioning fractions, soil C:N ratios. The soil partitioning and C:N ratios were kept as default. The microbial activity parameters were adjusted to minimize RMSE for N_2O and CO_2 emissions. The rainfall intensity multiplier for microbial activity was turned off. This should only be needed if the model is systematically underestimating soil water content.

4.2.5 Statistics

It is common to use statistical methods with defined criteria to compare the performances between models. Root mean square error (RMSE) and coefficient of determination (R^2) are two of the most commonly used statistics to access the “goodness of fit” of a model in predicting GHG emissions. To compare the performance ofthe models, three statistics from different perspectives were selected, including the percent bias (PBIAS), relative root mean square error (RRMSE) and correlation coefficient (R^2). PBIAS presents the difference in mean simulated and observed values, and it is considered satisfactory when it’s within $\pm 15\%$. A value of RRMSE $\leq$ 0.3 is usually considered as acceptable. The $R^2 = 1$ indicates perfect model performance, and we consider that the model performs satisfactorily when $R^2 > 0.5$. However, it is not always straightforward to judge model performance by only these criteria when modelling daily N_2O and CO_2 emissions, because they only indicate how models perform in a certain day (Giltrap et al., 2010). Model performance may be judged as “poor” if the predicted peak emission presents earlier or later than field measurements. A model should still be considered as promising when it predicts the cumulative emissions under different conditions because the seasonal cumulative emissions are the major concern in real situations. The detailed equations of the four statistics are shown as:

$$\text{PBIAS} = \frac{\sum_{i=1}^{n}(O_i - P_i)100}{\sum_{i=1}^{n} O_i} \qquad [4.7]$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(P_i - O_i)^2}{n}} \qquad [4.8]$$

$$\text{RRMSE} = \frac{RMSE}{\bar{O}} \qquad [4.9]$$

$$R^2 = \frac{\sum_{i=1}^{n}(O_i - \bar{O})(P_i - \bar{P})}{\sqrt{\sum_{i=1}^{n}(O_i - \bar{O})^2 \sum_{i=1}^{n}(P_i - \bar{p})^2}} \qquad [4.10]$$

Where P_i and O_i are the model predicted and experimental observed points. The total number of observations is n and $\overline{O}$ is the average observed value.

4.3 Results and discussion

4.3.1. Soil temperature

In terms of statistics, DNDC performed better than RZWQM2 in predicting the soil temperature (Table 4.5). Predictions of soil temperature using RZWQM2 agreed well with observations in all four treatments. RZWQM2 under-estimated soil temperature by 7 to 18%, mainly because RZWQM2 used air temperature as the boundary condition for the soil surface (Fang et al., 2015). In addition, it may also have underestimated temperature because it simulated temperature as an average daily value whereas measurements were taken around noon. Overall, RZWQM2 reasonably simulated soil temperature with RMSEs ranging from 2.8 to 5.0 ^oC, RRMSE from 20% to 25%, and R^2 from 0.70 to 0.74 for all the four treatments (Table 4.5).

DNDC performed better than RZWQM2 for the two treatments with PBIAS ranging from 2 to 8%, RMSEs from 2.5 to 2.7 ^oC, RRMSE varied from 13% to 14%, and R^2 from 0.88 to 0.93. Model performance of DNDC for predicting soil temperature in this study was comparable to the previous study at the same site from 2003 to 2005 by Li et al. (2017). Although RZWQM2 tended to miss most high peaks, both models simulated soil temperature dynamics reasonably well as compared with the measurements from 2012 to 2015 (Figure 4.1).

4.3.2. Soil water content

Although both RZWQM2 and DNDC reasonably simulated the SWC within the acceptable range (Table 4.6), RZWQM2 showed better performance with lower RRMSE and higher R^2. RZWQM2 simulations of daily SWC from 0 to 6 cm followed similar trends as measured values for all four treatments from 2012 to 2015 in the growing seasons except in 2012 under CDS system (Figure 4.2a). It greatly over-estimated the SWC when sub-irrigation was supplied in July and August. Overall, it performed satisfactorily in predicting SWC with average predicted values within 8% of observations, RRMSE from 0.14 to 0.19, and R^2 from 0.56 to 0.76 for all the four treatments (Table 4.6). Compared to RZWQM2, the DNDC model performed less satisfactorily in predicting the trends in SWC (Figure 4.2b). Although the PBIAS was within 3% and the RRMSE was within 18%, the R^2 (0.51 to 0.56) was lower than RZWQM2 for DR-IF and DR-SCM systems (Table 4.6).

Both RZWQM2 and DNDC simulated daily SWC driven by precipitation. Smith et al. (2017) compared RZWQM2 and DNDC in simulating SWC and daily water flow, indicating that DNDC needed improvements to include the algorithms for simulating root distribution, heterogeneous soil profile and water table. For soil water redistribution, the Richards equation was used in RZWQM2, while DNDC used an adapted cascade model (Frolking et al., 1998). Kröbel et al. (2010) compared the simulated soil water dynamics in North China Plain using DNDC and DAISY (Richards equation). They concluded that the Richards equation provided a better approximation of SWC than did the cascade flow used in DNDC Note that DNDC was not found to be sensitive to hydraulic conductivity. We also found this to be the case except during very high precipitation or irrigation events where ponding occurs. Otherwise, DNDC tips to field capacity on an hourly basis, ignoring hydraulic conductivity.

4.3.3 Drainage

The precipitation was 383.8, 604.3, 556.2 and 606.0 mm during the growing seasons (May to October) of 2012, 2013, 2014 and 2015, respectively. In general, RZWMQ2 performed well in predicting daily drainage under both DR and CDS systems during all four growing seasons and

DNDC simulated reasonable drainage under DR, even though it did not include a mechanistic approach for computing tile drainage (Table 4.7).

RZWQM2 performed satisfactorily in simulating daily drainage during the growing seasons under both free drainage and controlled drainage with sub-irrigation. The statistics of PBIAS, RRMSE and R^2 ranged from -14 to 14%, 0.06 to 0.10, and 0.67 to 0.87, respectively (Table 4.7). The measured daily drainage flow rates and those simulated by RZWQM2 are plotted in Figure 4.3a. The model correctly predicted less drainage under CDS than DR, since a higher water table was maintained under the CDS system. In the growing season of 2012, due to extremely low rainfall, almost no drainage was observed or simulated in all treatments even when sub-irrigation was applied in the CDS system. In 2014, RZWQM2 missed some drainage events in August and September for all treatments. The observed high peak after September 10^{th} was attributed to the high rainfall (72 mm) event on that day, however, the model didn't catch these peaks because of the over-estimation of runoff (simulated 29 mm VS 4 mm observed in DR-IF). Overall, our results for predicting daily drainage under controlled drainage with sub-irrigation was improved over the previous study using RZWQM2 by Lu (2015), who reported an over-estimation of total period drainage by 25% in the same experimental site from 2009 to 2011.

Although DNDC does not include a tile drainage component, it also performed satisfactorily in predicting the total drainage within 13% error with the R^2 value at 0.54 because the simulated drainage was highly relevant to precipitation. However, it showed poorer performance in estimating daily drainage than RZWQM2 did under DR-IF (R^2=0.54 and RRMSE=0.18). DNDC does not include an explicit tile drainage submodel thus neither drain spacing nor drain depth affects drainage. The hydraulic components that DNDC considers include precipitation, irrigation, soil and leaf evaporation, sublimation, crop transpiration, leaching and runoff. The only parameters available to calibrate drainage in DNDC are soil physical properties and crop water uptake. Li et al. (2006) developed a version of DNDC which could mimic tile drainage using a recession curve approach and Tonitto et al. (2007) modified four drainage parameters to improve simulation using this model version. However, this code is no longer active in the recent version of DNDC, and the parameters used by Tonitto et al. (2007) are not adjustable in the interface. In this study, we calibrated the parameters of crop water demand to adjust the evapotranspiration and thereby to match the daily drainage flow in the growing season.

4.3.4 Crop yield

Both RZWQM2 and DNDC accurately predicted corn and soybean yields under different N fertilizer applications within 15% error, and were able to correctly predict the low corn yield in 2014 due to late planting, after adjusting the corn parameters in terms of thermal degree days for maturity (Table 4.8).

RZWQM2 reasonably simulated the corn and soybean yield under four treatments all within 15% when compared with measured crop yield. It predicted 10% higher corn yield in CDS than DR system in the year of 2012, due to higher water supply from sub-irrigation and less water loss from drainage under CDS. The measured corn yield under CDS was expected to be higher than DR during the extremely dry growing season in 2012 (383.8 mm rainfall from May to October), however, there was no significant difference ($p>0.05$) between the measured corn yields under DR and CDS. Low precipitation in May (65.5 mm) and June (17.2 mm) was the major contributor for the dry growing season, meanwhile the SWC was reduced from around 0.3 cm^3 cm^{-3} to 0.2 cm^3 cm^{-3}. Water storage was correspondingly reduced by 10 mm in the top 10 cm of the soil profile. RZWQM2 might have over-estimated water stress in late July and August, since predicted water stress mainly occurred during the grain filling period, while in actuality crop water uptake appears to have been satisfied by soil water storage and rainfall as sufficient water was supplied from rainfall in July (102 mm) and August (110 mm).

4.3.5 N_2O emissions

RZWQM2 estimated cumulative N_2O emissions within 6% for all the four treatments and DNDC reasonably predicted the N_2O emissions within 8% under DR-IF and DR-SCM. However, both models had difficulties in predicting the timing and amount of peak N_2O fluxes with R^2 ranging from 0.37 to 0.51. Although RZWQM2 and DNDC had comparable performance in predicting N_2O flux in terms of R^2 and RMSE (Table 4.9), they simulated significantly different patterns in N_2O emission during the unmeasured periods (Figure 4.4). DNDC simulated more high peaks, while RZWQM2 predictions were more constant. For example, the DNDC predicted N_2O emission right after fertilization on May 16th, 2012 was 1036 g N ha^{-1}, which was 201 times greater than RZWQM2 (5.14 g N ha^{-1}) under DR-IF. However, since the peak values were simulated on the days when no measurements were taken, the possibility of these high emission peaks could not be verified in this study. Therefore, it is suggested to take more frequent measurements after fertilization to verify GHG emission and model performances.

The measured N_2O emissions for corn was lower under IF than SCM, while the condition was totally opposite for soybean. This is because there were higher soil nitrate and ammonium concentrations in IF plots than SCM for corn. Thus, the total nitrification and denitrification for corn was higher than for soybean. However, the total available N in the soil profile was higher for soybean under SCM than IF treatments due to the slow decomposition of soil cattle manure under corn and more total N input under SCM than IF, while most NH_4^+ was nitrified and NO_3^- was denitrified or absorbed by crops in the IF plots for corn. RZWQM2 successfully predicted lower N_2O emission under SCM than IF for corn and higher N_2O emission under SCM than IF for soybean. Similarly, the DNDC model also predicted less N_2O emission under SCM in 2012 and 2014 but more N_2O emission under SCM than IF in 2013 and 2015.

Both observed average N_2O emissions and those simulated with RZWQM2 under CDS were higher than DR. Similar findings were reported by Nangia et al. (2013), who demonstrated 19% higher N_2O emission under controlled drainage than conventional drainage from a four-year field experiment in Eastern Ontario. The higher N_2O emission under CDS than DR in our study was due to higher soil moisture content leading to more N_2O emission from denitrification. Our results are supported by previous reports, such as Elder and Lal (2008), who indicated a positive correlation between N_2O flux and SWC, and Giltrap et al. (2010) also demonstrated that higher SWC enhanced N_2O from denitrification under anaerobic conditions.

Although RZWQM2 and DNDC showed comparable performance in simulating N_2O emissions under DF-IF, the magnitude of their simulated N dynamics varied significantly (Figure 4.5). The total simulated denitrification amount under DR-IF over four years was 7.2 and 2.4 kg N ha^{-1} for RZWQM2 and DNDC, respectively, and the simulated total nitrification was 297 and 165 kg N ha^{-1} for RZWQM2 and DNDC. Volatilization of N simulated by DNDC under DR-IF was 28 and 46 kg N ha^{-1} in 2012 and 2014, while RZWQM2 simulated values were only 11 and 5 kg N ha^{-1}. The extremely high volatilization predicted for 2014 may have contributed to the low nitrification estimated by DNDC. However, no measurements were taken to verify the NH_3 volatilization, thus we suggest measurements ofNH_3 volatilization after fertilization in the future.

Both models predicted higher denitrification in 2014 than 2012 due to more precipitation and higher soil moisture content during the growing season of 2014. The simulated denitrification using RZWQM2 was 3.4 and 7.8 g ha^{-1} day^{-1} on average during the growing seasons in 2012 and 2014, while DNDC simulated no denitrification during the grow season. Grant et al. (2016) measured the daily denitrification rate under free drainage and reported an average value of 6.5 g ha^{-1} day^{-1}. Lu (2015) adjusted the denitrification rate between 7 to 40 g ha^{-1} day^{-1} with 200 kg inorganic N application during the growing season (May to October) to reduce the N loss and match the simulated corn yield with measured values using RZWQM2 at the same site in Harrow. The simulated results from RZWQM2 in this study were comparable to studies from both Lu (2015) and Elmi et al. (2005), while DNDC simulated much lower total denitrification.

The complex processes of N_2O production and consumption were controlled by many interacting factors and N substrates exist in various forms such as NH_4^+, NO_3^-, NO_2^-, NH_3, N_2, and N_2O. Therefore, it is understandable that models have difficulty in predicting daily N_2O flux (Chirinda et al., 2011). Although the statistics for predicting daily N_2O emissions indicate that both RZWQM2 and DNDC had difficulties in predicting the timing of N_2O emission peaks, the cumulative emission amounts were still within the acceptable range under four different treatments for RZWQM2. In this study, RZWQM2 showed similar performance in predicting the cumulative N_2O emissions under DR-IF when compared with DNDC, and performed better than DNDC in predicting the N_2O emissions under DR-SCM. Smith et al. (2002 and 2008b) demonstrated the difficulties of DNDC in predicting the proper timing of N_2O emissions, though it could predict the seasonal magnitude of N_2O emissions correctly. Smith et al. (2008b) compared the performance of DNDC and DAYCENT in simulating the N_2O emission in Quebec City and Woodlsee under different N fertilization and tillage practices. The DNDC model performed better than DAYCENT in simulating the seasonal N_2O emissions, while both models had difficulty in simulating the daily N_2O flux.

It should also be noted that the two models predicted N_2O emissions very differently during winter months and spring thaw periods within the four years (Figure 4.4). Although no measurements were taken during winter or spring in our study, Tatti et al. (2017) observed N_2O emissions in winter in high latitudes due to enhanced denitrification, which could be attributed to the lower O_2 concentration and increased nutrients in soil with decreasing soil gas exchange, disruption of soil aggregates and microbial cells as results of soil freezing. Teepe et al. (2001) also observed increased N_2O emissions when soil temperature decreased from 10 to -6 ^oC. DNDC's ability to predict N_2O emissions from freeze-thaw cycles has been assessed by many investigators (Smith et al. 2002; Li et al., 2000; Norman et al., 2008; Kariyapperuma et al., 2011), and our simulated results from DNDC indicated high emissions in winter and spring freeze-thaw periods, while RZWQM2 did not predict obvious N_2O emissions in the same time. However, Foltz (2017) stated that the high N_2O emission peaks simulated by DNDC in late winter and early spring were not observed in a corn field in Colorado. This could be explained by the unfrozen soil condition due to warm soil temperatures in the field. Therefore, N_2O emissions from freezing soil Eastern Ontario region should be further investigated in the future.

4.3.6 CO_2 emission

Since the crops in the chambers were removed, root respiration was not taken into consideration in this study. RZWQM2 outperformed DNDC in predicting soil CO_2 emission under DR-IF and DR-SCM systems with the PBIAS ranging from 4 to 14%, RMMSE from 43% to 54%, and R^2 from 0.54 to 0.57 (Table 4.10), while the DNDC model had poor performance in simulating the soil CO_2 emission with RRMSE 62% to 79%, and R^2 from 0.23 to 0.31. RZWQM2 was able to catch the higher CO_2 emission peaks during the growing season in four years under different treatments, while DNDC always missed these peaks and over-estimated the emissions in June and early July. Measurement intensity after fertilization should be increased to further verify the CO_2 emission. Although the performance of DNDC was not as good as RZWQM2, our prediction of CO_2 emission under inorganic fertilization was comparable to the study by Li et al. (2017), who reported an accurate prediction of DNDC model in the same experimental site with the RMMSE ranging from 66.5% to 71.6% in the corn-soybean rotation system. Li et al. (2017) found that the crop parameters of TDD (thermal degree days), biomass fraction of roots and shoots were very sensitive to the soil CO_2 emission peaks and timing, thus these parameters were adjusted to match the CO_2 emission.

There was no significant difference ($p>0.05$) between measured CO_2 under DR and CDS with both inorganic fertilization and solid cattle manure. However, significantly higher ($p<0.01$) CO_2 was found with SCM application than IF under both DR and CDS systems. Both RZWQM2 and DNDC accurately predicted higher CO_2 emission under DR-SCM than DR-IF due to the supply of soil organic carbon in solid cattle manure (Figure 4.6). Both experimental and RZWQM2 simulated results showed that water table management has a limited impact on CO_2 emission, but SCM application would result in higher CO_2 emissions than inorganic fertilization due to higher organic carbon from manure. RZWQM2 under-estimated the CO_2 emission in CDS system in the growing season of 2012, which might be due to the over-estimation of SWC during the sub-irrigation period.

4.4 Summary and Conclusion

This study is the first evaluation of the newly added GHG component for RZWQM2 under both inorganic fertilizer and manure application. DNDC performed better than RZWQM2 in simulating soil temperature, which provides a sound basis for the prediction of GHG emissions. RZWQM2 also performed fairly well in simulating soil temperature with PBIAS within 17% and the over-estimation may be because RZWQM2 used a fixed boundary condition for the soil surface temperature. After model calibration, RZWQM2 performed better than DNDC in simulating SWC with PBIAS within 13%, RRMSE within 21%, and R^2 ranged from 0.55 to 0.68. Although DNDC estimated the average SWC within 3% and the RRMSEs were within 17%, the R^2 for both DR-IF and DR-SCM were lower than RZWMQ2. The lack of a heterogeneous soil profile and root density was the major limitation of DNDC for an accurate prediction of SWC. The computational Richards equation used in RZWQM2 performed very well but requires much more time for model execution. Both RZWQM2 and DNDC performed reasonably well in predicting tile drainage under the DR system, but RZWQM2 performed better than DNDC in simulating the peaks and daily trends, and RZWMQ2 had the capability to handle tile drainage simulation under controlled drainage with sub-irrigation. Both models closely predicted crop yield and biomass over the four-year study for all treatments. Although both models failed to predict the amount and timing of daily N_2O peak emissions, they provided reliable estimates of cumulative N_2O emissions under different treatments over four years. RZWQM2 also performed much better than DNDC in predicting the daily CO_2 emissions and provided reliable estimated of average CO_2 emission under different treatments.

Overall, RZWQM2 is an agricultural system model which comprehensively handles crop growth, hydraulic cycles and nutrient cycling at the field scale, and DNDC is specialized for nutrient cycling but also reasonably simulated SWC, drainage and crop growth. RZWQM2 requires very experienced users for calibration and validation due to the uncertainty and complexity of parameters and is more computationally intensive, while DNDC is more user-friendly and works well with simple calibration. It is important to test the hydraulic components of agricultural system models to better understand the complicated interaction between soil, water and nutrients. Improvements are suggested for DNDC in computing soil water dynamics. This could substantially impact C and N cycling and improve the temporal representation of drainage and GHG emission events. Further evaluations are needed to test RZWQM2 for predicting NH_3 volatilization, the methanogenesis process for CH_4 emissions and the impacts of organic and inorganic manure management on GHG emissions across a wider array of soils and climatic conditions.

Acknowledgement

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Table 4.1. Agronomic management from 2012 to 2015 (IF: inorganic fertilization; SCM: soil cattle manure)

Year	Crop	Sowing Date	Harvest Date	IF (kg N/ha)	SCM (kg N/ha)	
				NH_4NO_3	NH_4NO_3	Organic N
2012	Corn	25-May	5-Nov	200	130.84	230.55
2013	Soybean	16-May	9-Oct	0	0	0
2014	Corn	29-Jun	28-Nov	200	110.67	297.74
2015	Soybean	25-May	8-Oct	0	0	0

Table 4.2. Measured and calibrated soil hydraulic parameters.

Layer	Depth (m)	ρ (Mg m^{-3})	Soil Water Retention						Lateral k_{sat} (mm h^{-1})	Vertical k_{sat} (mm h^{-1})
			θ_s (m^3m^{-3})	FC33 (m^3m^{-3})	FC15 (m^3m^{-3})	θ_r (m^3m^{-3})	τb	λ		
1	0-0.05	1.36	0.487	0.233	0.104	0.025	-14.5	0.141	30	15
2	0.05-0.25	1.60	0.415	0.227	0.109	0.025	-24.1	0.180	60	30
3	0.25-0.45	1.46	0.449	0.330	0.248	0.025	-5.9	0.082	34	17
4	0.45-0.80	1.40	0.472	0.350	0.272	0.025	-3.9	0.072	20	10
5	0.80-1.20	1.40	0.464	0.328	0.246	0.025	-3.8	0.083	20	10
6	1.20-1.50	1.40	0.464	0.320	0.236	0.025	-3.5	0.087	20	10
7	1.50-2.00	1.40	0.464	0.250	0.166	0.025	-3.0	0.170	1	1

[a] ρ = bulk density, θ_s = saturated soil water content, FC33= field capacity at 1/3 bar, FC15= field capacity at 15 bar, θ_r = residual soil water content, τb = bubbling pressure, λ = pore size distribution index, k_{sat}=saturated hydraulic conductivity. Bulk densities are measured while others are calibrated values.

[b] Other required parameters include A1 (set to zero), B (computed using the RZWQM default constraint) for all layers, N_1 (set to zero), and K_2 and N_2 (computed using the RZWQM default constraints) for all layers (Ahuja et al., 2000b). The lateral hydraulic gradient was adjusted to a value of 1.5×10^{-6}.

Table 4.3. Calibrated hydrologic and nutrient parameters in RZWQM2

Non-default Parameters	Value
Hydrology component	
Minimum leaf stomatal resistance (s m^{-1})	150
Albedo of dry soil	0.2
Albedo of wet soil	0.3
Albedo of crop	0.3
Albedo of fresh residue	0.3
Drain depth (m)	0.85
Drain spacing (m)	3.8
Radius of drain (cm)	7.6
Surface soil resistance for S-W	250
Water table leakage rate (cm hr^{-1})	0.0001
Nutrient component	
Slow residue pool to intermediate soil	0.1
Fast residue pool to Fast soil humus pool	0.3
Fast soil humus pool to intermediate soil	0.6
Intermediate soil to slow soil humus pool	0.7
Decay rate of slow residue pool	1.673×10^{-8}
Decay rate of fast residue pool	5.14×10^{-8}
Decay rate of fast soil humus pool	5.5×10^{-7}
Decay rate of intermediate soil humus pool	5×10^{-7}
Decay rate of slow soil humus pool	4.7×10^{-9}
Denitrification rate	2.0×10^{-14}

Table 4.4. Calibrated and measured (*) soil and crop parameters in the DNDC model

Soil Parameters		Value
Soil pH*		5.4
Field capacity (wfps)		0.72
Wilting point (wfps)		0.4
Clay fraction*		0.37
Conductivity (cm hr^{-1})		1.5
Soil initial C*		1.66%
Porosity*		0.449
Crop parameters	Corn	Soybean
Maximum grain biomass production (kg C/ha/year)	6500	3200
Biomass C: N ratio (grain)	45	10
Biomass C: N ratio (leaf)	80	45
Biomass C: N ratio (stem)	50	40
Biomass C: N ratio (root)	40	20
N fixation index	0	1
Water demand (g water/g dry matter)	125	330
Thermal degree days for maturity	2950	1800
Microbial activity parameters		
Rainfall Intensity multiplier for microbial activity (1 default)		0 (off)
Denitrifier Growth rate activity (1 default)		0.70
Nitrifier Growth rate activity (1 default)		0.25

Table 4.5. Statistics for evaluating model performances in soil temperature simulations (0 to 6cm)

Model	treatment	Obs ºC	Sim ºC	PBIAS	RMSE ºC	RRMSE	R^2
RZWQM	DR-IF	18.0	16.8	7%	2.8	0.23	0.73
	DR-SCM	20.0	16.8	16%	4.7	0.23	0.70
	CDS-IF	19.1	16.7	12%	3.7	0.20	0.74
	CDS-SCM	20.4	16.8	18%	5.0	0.25	0.72
DNDC	DR-IF	18.0	19.6	-8%	2.5	0.14	0.93
	DR-SCM	20.0	19.6	2%	2.7	0.13	0.88

Table 4.6. Statistics for evaluating model performance in soil water content (SWC) simulations (0 to 6 cm)

Model	treatment	Obs $cm^3\ cm^{-3}$	Sim $cm^3\ cm^{-3}$	PBIAS	RMSE $cm^3\ cm^{-3}$	RRMSE	R^2
RZWQM2	DR-IF	0.27	0.25	5%	0.04	0.15	0.64
	DR-SCM	0.26	0.26	2%	0.04	0.14	0.76
	CDS-IF	0.26	0.28	-8%	0.05	0.19	0.64
	CDS-SCM	0.29	0.29	-1%	0.06	0.18	0.56
DNDC	DR-IF	0.27	0.27	0%	0.05	0.18	0.51
	DR-SCM	0.26	0.27	-3%	0.05	0.18	0.56

Table 4.7. Statistics for evaluating model performance in daily drainage flux simulation

Model	treatment	Obs (mm)	Sim (mm)	PBIAS	RMSE (mm)	RRMSE	R^2
RZWQM2	DR-IF	0.41	0.47	14%	0.04	0.10	0.87
	CDS-IF	0.18	0.19	7%	0.01	0.07	0.67
	CDS-SCM	0.28	0.24	-14%	0.02	0.06	0.81
DNDC	DR-IF	0.41	0.47	13%	0.07	0.18	0.54

Table 4.8. Measured and simulated crop yield (Mg ha^{-1})

		DR-IF			CDS-IF			DR-SCM			CDS-SCM		
crop	year	obs	sim		obs	sim		obs	sim		obs	sim	
RZWQM	2012	11.4	11.7	-3%	10.9	12.4	-14%	11.2	11.2	0%	11.4	12.4	-8%
	2013	4.1	4.0	4%	3.6	3.6	1%	4.0	4.0	2%	3.6	3.6	-3%
	2014	3.9	4.0	-4%	3.9	4.0	-3%	4.1	4.1	2%	4.1	4.1	2%
	2015	3.5	3.9	-13%	3.5	3.8	-9%	4.2	4.0	5%	3.5	3.9	-15%
DNDC	2012	11.4	11.1	2%				11.2	10.9	3%			
	2013	4.1	4.1	-1%				4.0	4.1	2%			
	2014	3.9	4.1	-6%				4.1	4.1	0%			
	2015	3.5	3.9	-10%				4.2	3.9	8%			

Table 4.9. Statistics for evaluating model performance in soil N_2O emissions simulation

Model	treatment	Obs g N ha^{-1}	Sim g N ha^{-1}	PBIAS	RMSE g N ha^{-1}	RRMSE	R^2
	DR-IF	2.42	2.30	5%	3.00	1.24	0.47
	DR-SCM	2.66	2.64	1%	2.90	1.09	0.48
	CDS-IF	3.15	3.28	-4%	5.26	1.67	0.40
RZWQM2	CDS-SCM	2.61	2.76	-6%	4.25	1.63	0.37
	DR-IF	2.42	2.31	4%	2.90	1.20	0.46
DNDC	DR-SCM	2.66	2.86	-8%	2.66	1.00	0.51

Table 4.10. Statistics for evaluating model performances in soil CO_2 emissions simulations

Model	treatment	Obs kg ha^{-1}	Sim kg ha^{-1}	PBIAS	RMSE kg ha^{-1}	RRMSE	R^2
	DR-IF	13.1	12.8	4%	5.6	0.43	0.57
	DR-SCM	17.8	20.3	-14%	9.6	0.54	0.54
	CDS-IF	12.6	13.3	-6%	7.4	0.59	0.33
RZWQM2	CDS-SCM	17.3	19.5	-13%	9.3	0.54	0.34
	DR-IF	13.1	13.9	-4%	8.1	0.62	0.31
DNDC	DR-SCM	17.8	16.3	8%	14.0	0.79	0.23

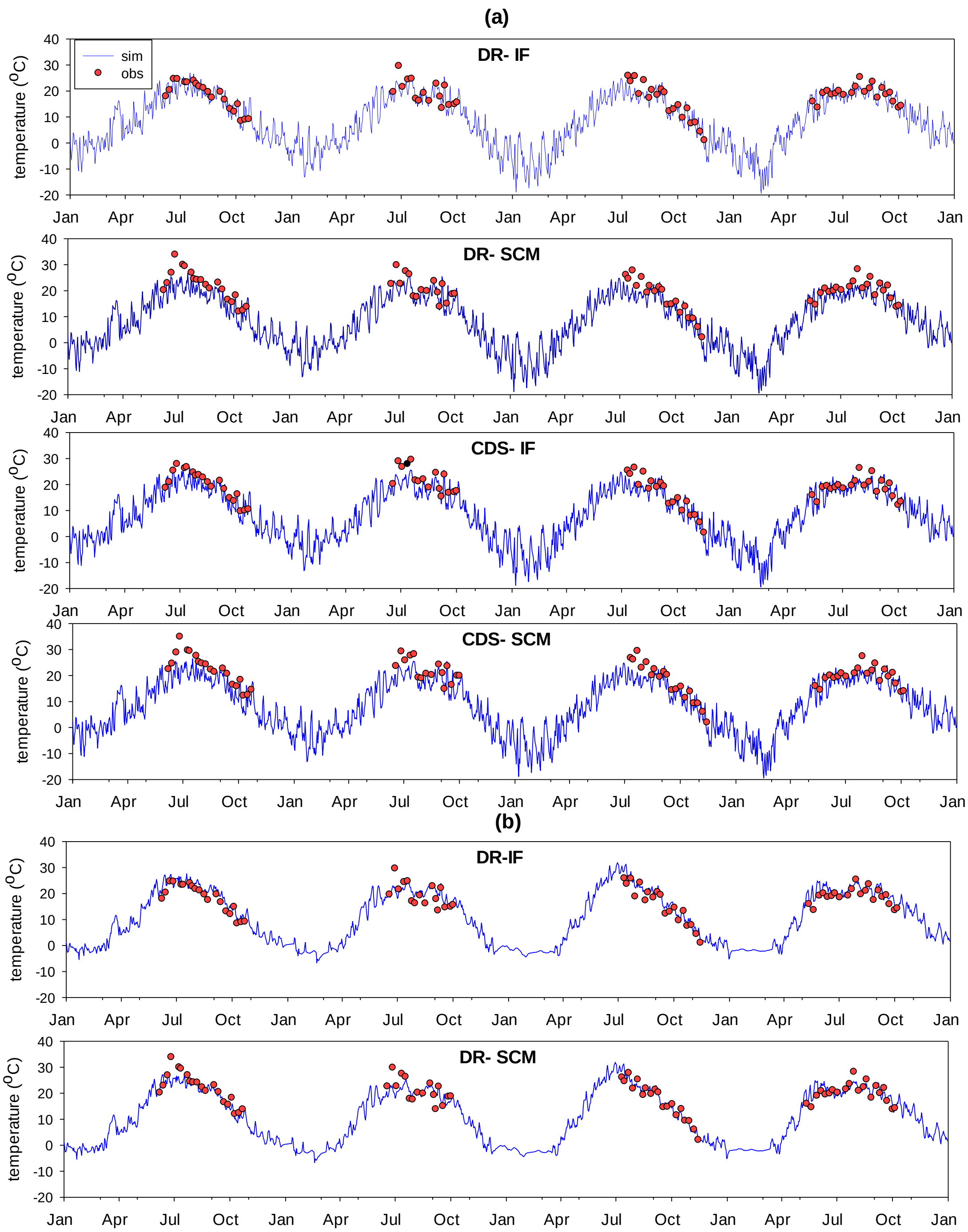

Figure 4.1. Comparison of field measured, (a) RZWQM2 simulated and (b) DNDC model simulated soil temperature at the soil depth of 6 cm.

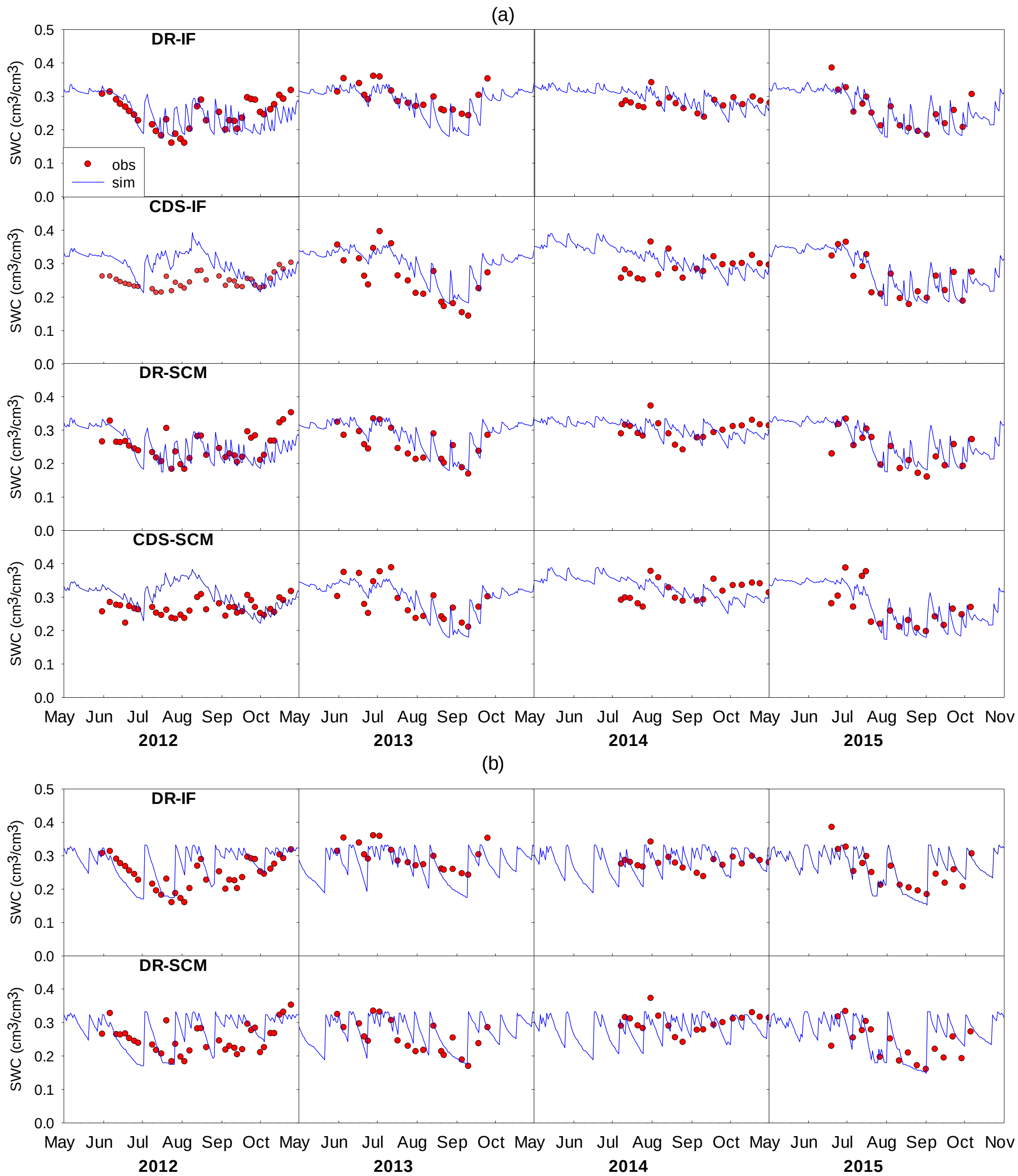

Figure 4.2. Comparison of field measured, (a) RZWQM2 simulated and (b) DNDC simulated soil water content (SWC)

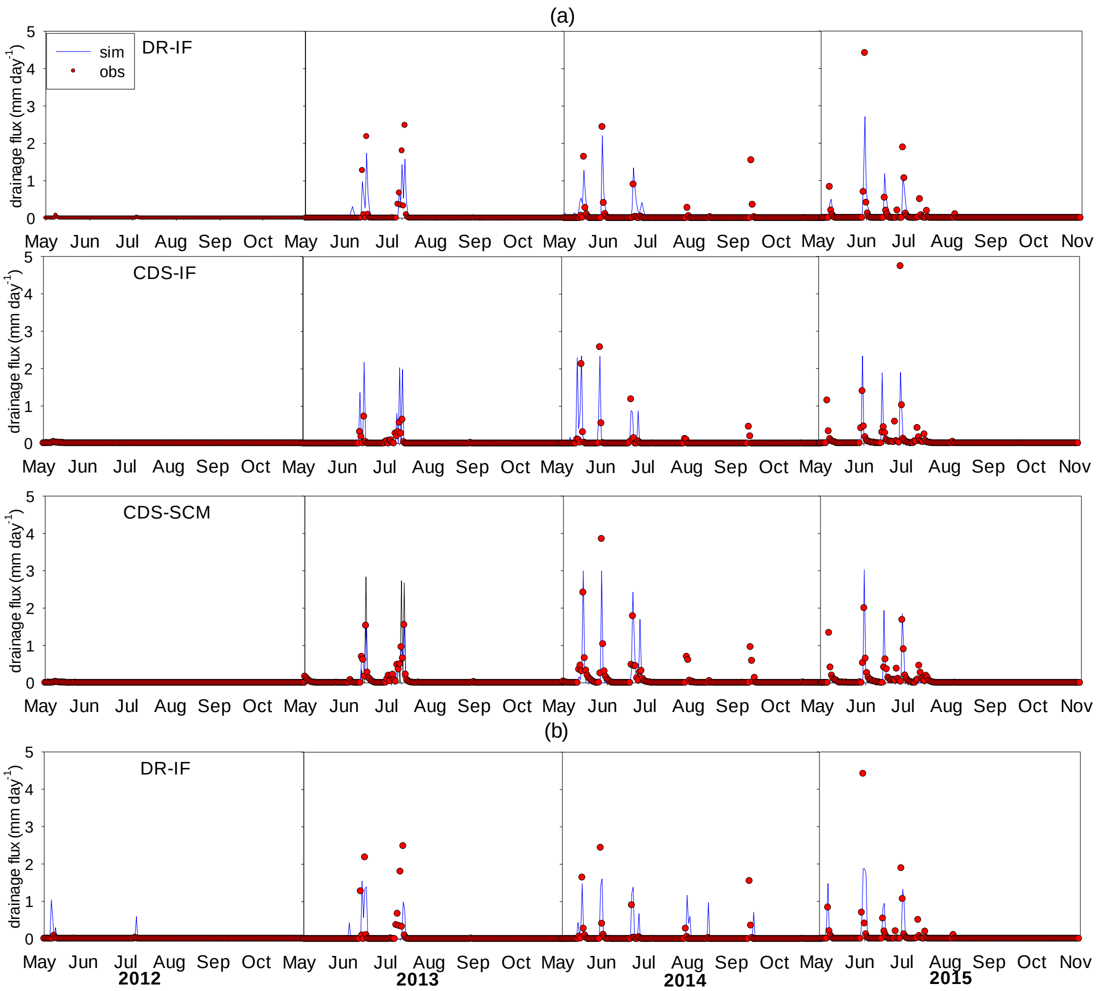

Figure 4.3. Comparison of field measured, (a) RZWQM2 simulated and (b) DNDC simulated daily drainage flux during the growing season from 2012 to 2015

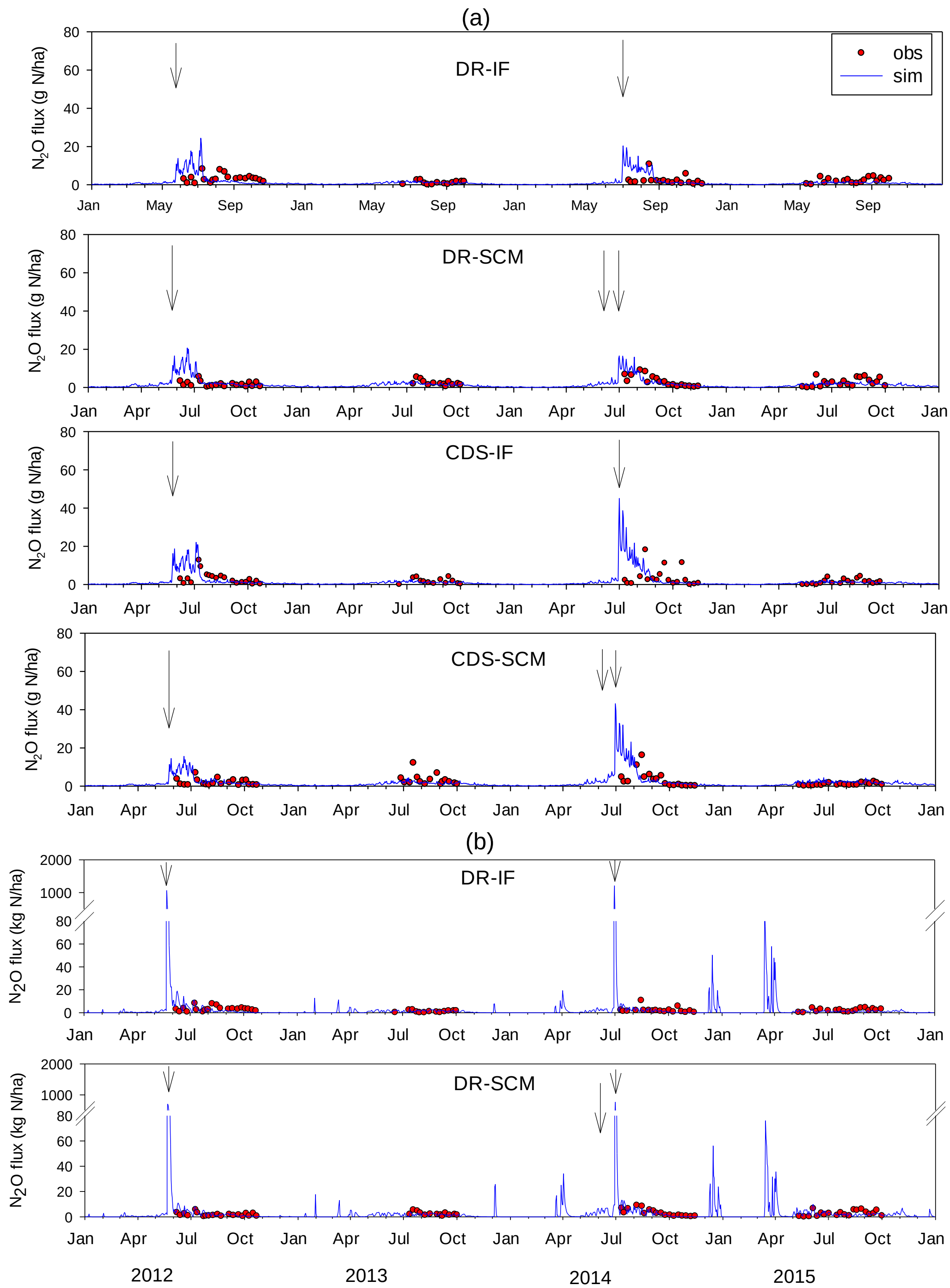

Figure 4.4. Measured and simulated N_2O emissions by (a) RZWQM2 and (b) DNDC under DR-IF (Arrows are fertilizations)

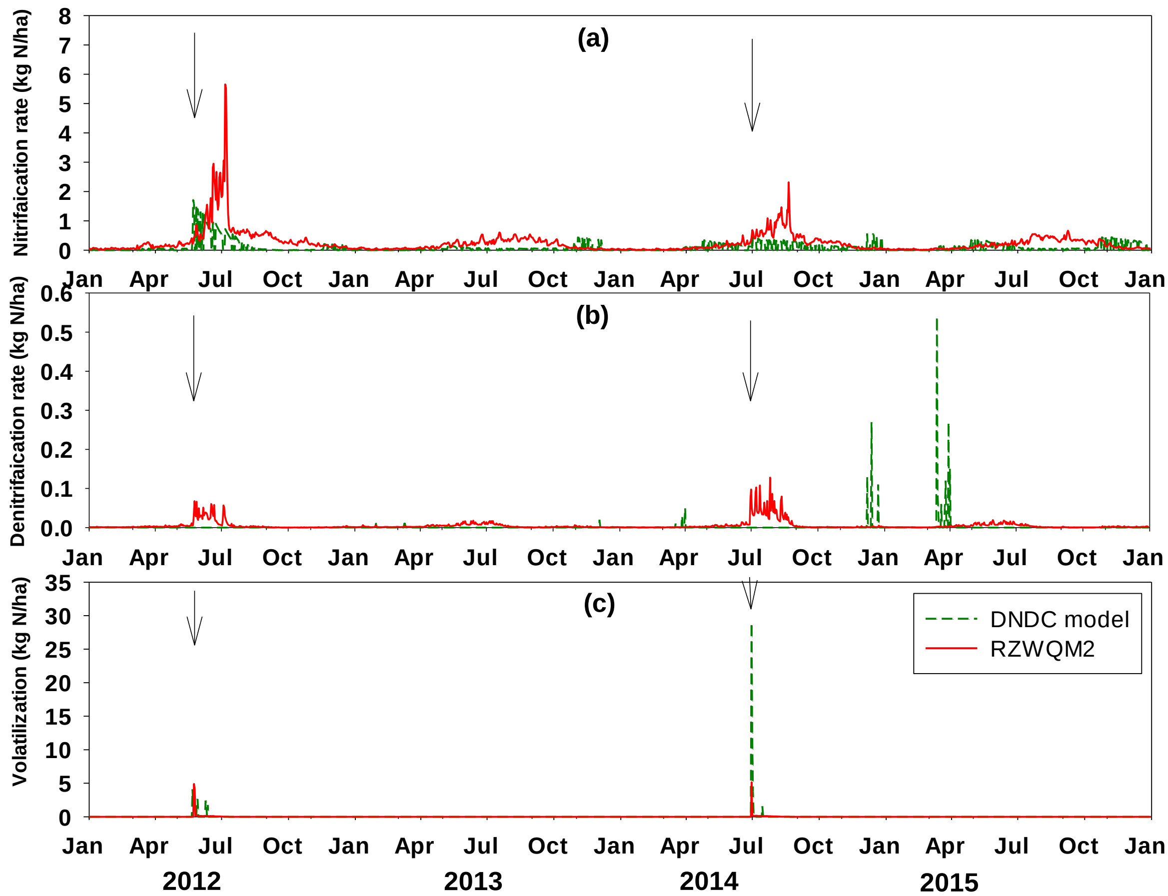

Figure 4.5. Simulated daily (a) nitrification and (b) denitrification in soil profile by DNDC and RZWQM2 under DR-IF system (Arrows are fertilizations)

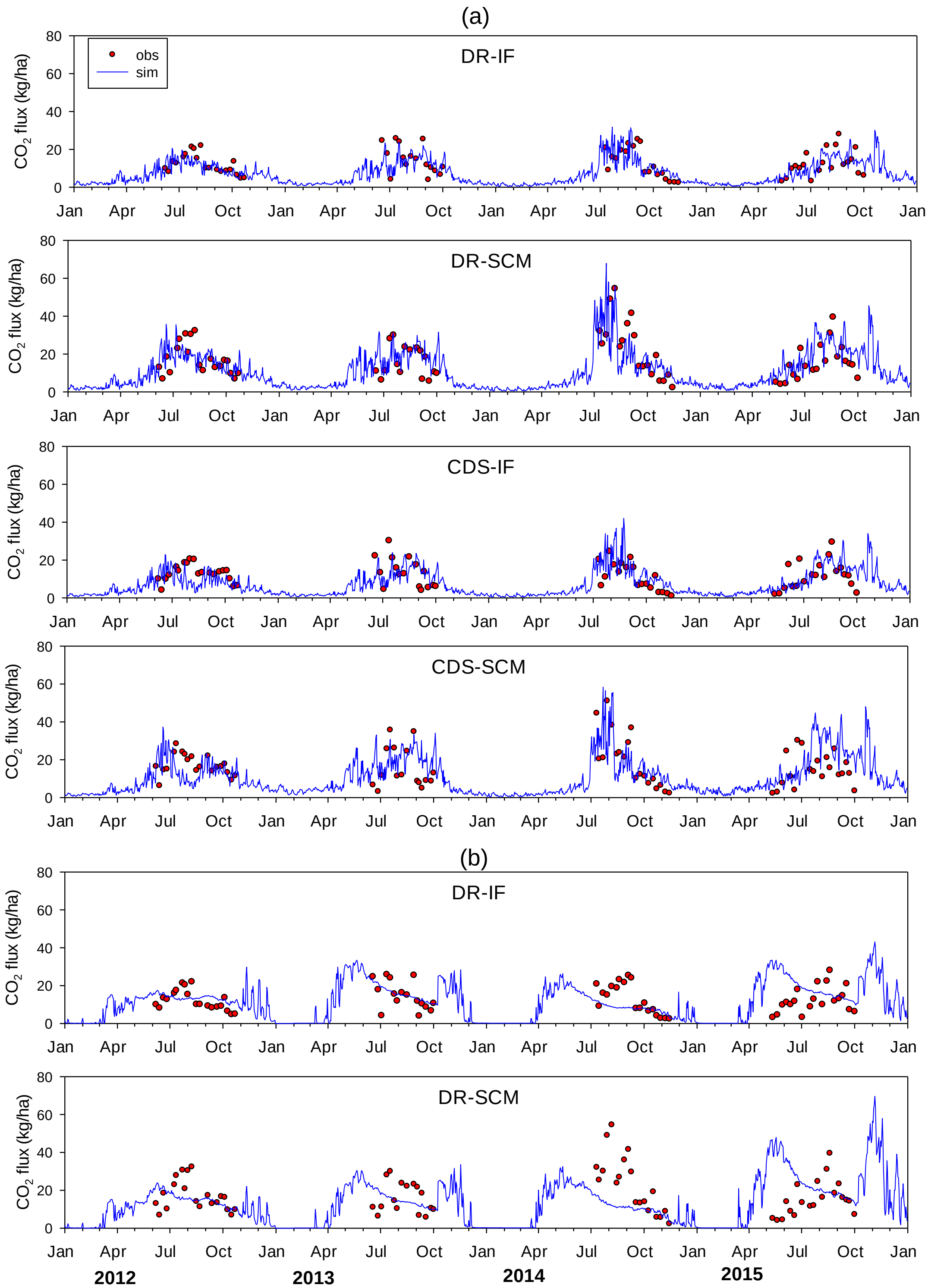

Figure 4.6. Measured and simulated CO_2 emission by (a) RZWQM2 and (b) DNDC

Connecting text to Chapter 5

Chapter 4 testedRZWQM2 by comparing its performance with a C:N cycling model, DNDC, in simulating the comprehensive biochemical processes in the soil profile and crop growth. RZWQM2 was found to have comparable performance with DNDC in predicting N_2O emissions but was better than DNDC for simulating CO_2 emissions. It has better algorithms for soil water dynamics and tile drainage simulation. It was more applicable for simulating the GHG emissions and hydraulic components in sub-surface drained fields. This chapter reports further testing of the nutrient component of RZWQM2 for predicting the GHG emissions under water table management using four years' measured N_2O and CO_2 emission data. After model evaluation, a few agronomic management practices were implemented using the model to investigate their long-term impact on GHG emissions, and thereby some suggestions were proposed to mitigate GHG emissions from agricultural soils. The following manuscript, co-authored by Dr. Zhiming Qi, Dr. Chandra Madramootoo and Cynthia Crézé, has been published in the journal of Science of the Total Environment.

Jiang, Q., Qi, Z., Madramootoo, C.A. and Crézé, C. 2019. Mitigating greenhouse gas emissions in a subsurface-drained field in Southern Quebec using RZWQM2. Science of the total environment, 646, 377-389.

Chapter 5

Mitigating greenhouse gas emissions in a subsurface-drained field in Southern Quebec using RZWQM2

Qianjing Jiang, Zhiming Qi, Chandra A. Madramootoo, Cynthia Crézé

Abstract

Greenhouse gas (GHG) emissions from agricultural soils are affected by various environmental factors and agronomic practices. The impact of inorganic nitrogen (N) fertilization rates and timing, and water table management practices on N_2O and CO_2 emissions were investigated to propose mitigation and adaptation efforts based on simulated results founded on field data. Drawing on 2012-2015 data measured on a subsurface-drained corn (*Zea mays* L.) field in Southern Quebec, the Root Zone Water Quality Model 2 (RZWQM2) was calibrated and validated for the estimation of N_2O and CO_2 emissions under free drainage (FD) and controlled drainage with sub-irrigation (CD-SI). Long term simulation from 1971 to 2000 suggested that the optimal range of N fertilization should be in the range of 125 to 175 kg N ha^{-1} to obtain higher NUE (nitrogen use efficiency, 7-14%) and lower N_2O emission (8-22%), compared to 200 kg N ha^{-1} for corn-soybean rotation (CS). While remaining crop yields, splitting N application would potentially decrease total N_2O emission by 11.0 %. Due to higher soil moisture and lower soil O_2 under CD-SI, CO_2 emissions declined by 6% while N_2O emissions increased by 21% compared to FD. The CS system reduced CO_2 and N_2O emissions by 18.8% and 20.7%, respectively, when compared with continuous corn production. This study concludes that RZWQM2 model is capable of predicting GHG emissions, and simulations suggest that GHG emissions from agriculture can be mitigated using agronomic management practices.

Key words: Controlled drainage; N management; water table management; GHG mitigation; rotation

5.1 Introduction

Greenhouse gas (GHG) is an important factor for global climate change, due to the great impact of the three major GHGs, nitrous oxide (N_2O), carbon dioxide (CO_2) and methane (CH_4) on regulating precipitation and temperature (Ozlu and Kumar, 2018). Agricultural activities are significant contributors for GHG emissions. Approximately 8% of total GHGs are emitted directly from agriculture, since 52% and 84% of global CH_4 and N_2O emissions are produced from agriculture and agricultural soils act as both sink and source for CO_2 (Smith et al., 2008a). In developing countries, GHG emissions arising from agricultural activities increased 32% between 1990 and 2005, and continues to do so in the face of rising population and food demands (IPCC, 2014). Reducing GHG emissions, mitigating the effects of GHG emissions and adapting to changes in climate without reducing food production and jeopardizing food security is becoming a global challenge.

Nitrous oxide emissions arise from nitrification under aerobic conditions, or denitrification under anaerobic conditions, and carbon dioxide is mainly released through the aerobic decomposition of soil organic carbon. In an agricultural context, the extent and nature of GHG emissions is closely related to the pH, temperature, moisture content and the nutrient availability of the cultivated soil (Oertel et al., 2016). Agronomic management affects GHG emissions by altering soil nutrients, and the aerobic or anaerobic conditions to which microorganisms are exposed. It was reported that the inorganic N fertilization accounts for 22% to the total GHG emissions from agriculture in Canada (ECCC, 2017). Tile-drained fields were reported to produce 45% less N_2O emissions from soil than undrained fields in Wells, MN (Fernández et al., 2016). Controlled drainage reduces drainage outflow and enhances denitrification, thereby reducing NO_3^--N losses (Ridao et al., 1998), however, it also results in more N_2O release from denitrification (Kliewer and Gilliam, 1995), due to higher soil water content (SWC) under water table management. Elder and Lal (2008) indicated a positive correlation between N_2O flux and SWC, since higher SWC enhanced the N_2O arising from denitrification under anaerobic conditions (Giltrap et al., 2010). Andrade et al. (2002) demonstrated that when dissolved organic carbon was added to sub-irrigation water applied under controlled drainage, the bacterial denitrification process which transforms N_2O to N_2 was enhanced, NO_3^- pollution was lowered, and less N_2O was released to the atmosphere. In reducing GHG emissions from agricultural soils, one must optimize crop fertilization, as not all crops can take up all forms of N, and forms or methods of N fertilization which do not favor plant uptake could result in more N_2O emissions (McSwiney and Robertson, 2005) and N leaching (Bergström and Brink, 1986). To mitigate the GHG emissions, some agronomic management practices were suggested, such as precision fertilization by estimating the crop N required to avoid excess N application, the use of rotations with legume crops, cover crops, and optimizing the timing of N application to improve N use efficiency (Smith et al., 2008a). Others have reported that cover crops could increase CO_2 and N_2O emissions (Sanz-Cobena et al., 2014), and tillage could also enhance GHG emissions (Omonode et al., 2011, Gillette et al., 2017b) because it improves soil porosity, thereby raising the soil O_2 concentration ($[O_2]_{soil}$) and promoting the aerobic activities of nitrification and respiration.

N_2O emissions show great variability corresponding to spatial and timing with changing soil environment, because the soil temperature, soil moisture content, soil N and O_2 availability are all affected by the climate condition and agricultural activities (Fang et al., 2015). Although field experiments have been conducted to measure GHG emissions, collecting the GHG emission data on a daily basis over the long term has been laborious and very costly. Computer modeling allows for the simulation of GHG emissions over a longer time period. In addition, computer modeling provides the possibility to assess the effects of various agronomic practices on GHG emissions and crop production. A numbers of process-based models have been developed and evaluated for estimating GHG emissions (Giltrap et al., 2010, Hashimoto et al., 2011, Li et al., 2015). One such model, the DNDC (Denitrification–Decomposition) model is capable of simulating N_2O, CH_4, and CO_2 emissions, and has been tested in the United States (Li, 1995; Tonitto et al., 2007) , Canada (Smith et al., 2002), India (Pathak et al., 2005), China (Cai et al., 2003), and Europe (Levy et al., 2007). However, the DNDC model does not have a tile drainage component, and it is not able to simulate the impact of controlled drainage or subirrigation on GHG emissions.

The Root Zone Water Quality Model (RZWQM2) is a comprehensive one-dimensional field-scale model which can be used to study the interaction of physical, chemical, and biological processes within the soil profile, including the movement of water, nutrients, pesticides as well as crop growth under various management practices (Ahuja et al., 2000b). Optional management practices include controlled drainage, different types of irrigation, inorganic and manure fertilization, tillage, pesticide, cover crop and crop rotations. Fang et al. (2015) improved the RZWQM2 model after comparing the performance of four N_2O emission algorithms (*i.e.*, DAYCENT, NOE, WNMM, and FASSET) by coupling them with RZWQM2 to predict N_2O emissions from soil nitrification and denitrification processes. These algorithms of N_2O emissions from nitrification in NOE and N_2O release from denitrification in DAYCENT were then added to the RZWQM2. In testing the modified RZWQM2 model's ability to predict the effect of tillage and N fertilizer application rate on N_2O emissions in an irrigated corn (*Zea mays* L.) field in Colorado, Gillette et al. (2017b) found that conventional tillage led to 10% (simulated) and 12% (measured) greater annual N_2O emissions than a no tillage treatment when a high rate of N fertilisation was applied. However, the model overestimated N_2O emissions by 16% under no-till low N fertilization rate treatments, but underestimated them by 10% under conventional tillage. Wang et al. (2016) applied the modified RZWQM2 model to test the possibility of different management practices (*e.g.*, N application rate, tillage system, new crop cultivars/lines, water table management practices, and planting date) to mitigate the adverse effects of climate change in Iowa, USA. Long-term simulation results suggested that new corn cultivars could contribute to increasing yields and reducing N_2O emissions and N losses in drainage in the future.

Calibrated and validated agricultural system models could evaluate agronomic management options to mitigate GHG emissions. In addition, models can estimate the annual and long term GHG emissions, which is difficult and costly to conduct by field experiments on a daily basis over a long time period. The RZWQM2 has been evaluated to simulate different tillage effects on N_2O emissions, but it has never been tested for simulating CO_2 emissions from agricultural soils. The objectives of this paper are to 1) test RZWQM2's ability to predict the emissions of two GHGs in a subsurface drained field under water table management; 2) use RZWQM2 to investigate the impacts of different agronomic management practices on long-term annual GHG emissions; 3) propose mitigation and adaptation suggestions based on the model simulations.

5.2 Methods and materials

5.2.1 Overview of RZWQM2

RZWQM2 is a one-dimensional agricultural system model capable of simulating the movement of water, nutrients and pesticides in agricultural soils, as well as crop growth under various management practices (Ahuja et al., 2000b). It houses subroutines dedicated to physical, chemical and biological processes of an agricultural system. The model uses the Green-Ampt equation (Green and Ampt, 1911) to simulate the infiltration of surface water and melted snow into the soil and the Richards equation to calculate water distribution in the soil profile between rainfall or irrigation events (Ahuja et al., 2000b). The potential evaporation (E_p) and crop transpiration (T_c) are described by the Shuttleworth-Wallace equation (Shuttleworth and Wallace, 1985). Tile drainage flux is calculated by the Hooghoudt equation (Hooghoudt, 1940). Agricultural management practices that are available for users include crop cultivar selection, planting date, manure application, irrigation, fertilization, pesticides, and tillage. In the case of sub-irrigation, water is introduced into the soil profile at a user-defined depth and handled as a source in the Richards equation.

The OMNI program, developed as a submodel of RZWQM2, simulates the organic matter and nitrogen cycling pathways, including mineralization and immobilization, inter pool transfer of C and N, aerobic nitrification, anaerobic decay and denitrification, microbial biomass growth and death, etc. In OMNI, the decayed soil organic carbon (SOC) is channeled in three directions: transfer to other organic matter pools, assimilation into biomass, or to a C sink *via* CO_2 generated from biomass respiration. Drawing on a fraction of the biomass pool lost to inter-pool transfer, OMNI converts the remaining decayed organic matter to biomass C by way of an efficiency factor, and considers the remaining organic C as going to a C sink as CO_2 from aerobic respiration (Ahuja et al., 2000b). The organic matter is divided into five pools: (i) plant or other organic structural material (slow pool), (ii) plant or other organic metabolic material (fast pool), including crop residues, manure, and other organic materials, (iii, iv, v) fast, medium and slow decaying SOM pools. The basic equations for computing the decomposition rates of different pools are the same, while the coefficients of decay for different pools are different, which are computed as a function of user-defined rate coefficient, microbial population size, the population of aerobic heterotrophic microbes, ionic strength, temperature, water filled pore space (WFPS)), O_2 concentration, etc. However, the CO_2 emissions from root respiration and assimilation by the plant from photosynthesis are not considered in this model. The algorithms for N_2O emissions from nitrification are adapted from the NOE model which computes the N_2O emission using a fraction of nitrification for N_2O emissions, a soil water factor for the oxygen availability and the quantity of nitrification, while N_2O release from denitrification is computed using algorithms from the DAYCENT model based on NO_3-N content, soil respiration, and water filled pore space. In RZWQM2, the OMNI program is linked to other sub-models for a comprehensive simulation of the whole system, including plant growth, soil chemistry, and solute transport.

5.2.2. Fields experiment

The field study was conducted from 2012 to 2015 at a 4.2-ha subsurface-drained corn field in the Saint-Emmanuel sector of Côteau-du-Lac, Quebec (lat. 45.32N, long. 74.17W). The soil at this site was a Soulanges very fine sandy loam with 5.0% organic matter in the top layer (0-0.25 m), followed by layers of sand clay loam with 1.5% organic matter (0.25-0.55 m) and a clay layer with little organic matter content (0.55-1.0 m). Yellow bean (*Phaseolus vulgaris* L.) was planted in 2012 and grain-corn was planted each of the next three years (Pioneer 9918 in 2013, Pioneer 9855 in 2014 and Pioneer 9917 in 2015). Each year inorganic N fertilization was applied prior to seeding and during the growing season at rates and dates shown in Table 5.1. Tillage practices were applied 24 hours before seedling using spring tooth harrow and after harvest with chisel plow each year.

The subsurface drains were installed on a 0.5% slope at a maximum depth of 1.0 m, lengthwise along each subsurface drained plot (75 m $\times$ 15 m; Madramootoo et al., 2001). These plots were grouped into three blocks, each housing two water table management regimes: conventional free drainage (FD) and controlled drainage with subirrigation (CD-SI). All plots were under FD for the first two years (2012 and 2013), while separate CD-SI and FD plots were implemented in 2014 and 2015 (Figure 5.1); data from the former served in the model validation, while data from the latter served in model validation. For CD-SI, the water table depth was maintained between 0.60 m to 0.75 m from the soil surface by means of pumping water from a well into the drainage pipes through a water control structure.

The GHG samples were taken from four chambers per block, with a total of three blocks (Figure 5.1) in 2012 and 2013. All chambers were under FD and in 2014 and 2015; two chambers in each block were under FD with the other two under CD-SI. The closed chambers (0.556 m $\times$ 0.556 m $\times$ 0.140 m), each equipped with a gas sampling and a vent tube port, were inserted into the soil to a depth of 0.10 m. Measurements of GHG fluxes were taken weekly during the growing season of the four years. Gas samples were taken using a 20-ml syringe with a needle tip (25-gauge, 1.6 cm, Benton and Dickson) at 0, 15, 30, 45 and 60 minutes from each chamber, and immediately placed in exetainers with 15 mg magnesium perchlorate (Labco, High Wycombe, UK) to absorb water vapor. Gas concentrations in all samples were analyzed in lab using the Bruker 450-GC System (Bruker corp., Bremen, Germany), then the non-steady-state diffusive flux estimator (NDFE) was applied to compute the gas fluxes from the changes of measured gas concentrations as described by Livingston et al. (2006). Detailed information on the procedure can be found in Crézé (2015).

Hourly air temperature, precipitation, relative humidity and wind speed were obtained from the Environment Canada weather station at Côteau-du-Lac (Station ID – 7011947), located 500 m from the experimental site. Soil physical and chemical properties including soil texture, organic matter content (SOM) and bulk density (ρ) were measured using undisturbed soil cores taken from the field. The temperature of the soil's top 0.06 m was monitored using a hand-held thermometer (Hanna® Instruments), while its volumetric water content (θ_v) was measured with a ThetaProbe (Model ML2x; Delta-T Devices Ltd., 1999, Cambridge, UK).

5.2.3 RZWQM2 Model calibration

The hydraulic component of the model was calibrated against the θ data measured under FD in 2012 and 2013, and validated using measured θ data from 2014 to 2015 under FD and CD-SI. The calibrated soil hydraulic parameters for different soil layers are listed in Table 5.2. Nutrient parameters were calibrated to match with the GHG emission measurements (Table 5.3). With the default organic matter decay rates, the model predicted large peaks after crop harvesting each year due to the fast decomposition of crop residue on soil surface. Therefore, decay rates of both slow and fast residue pools were decreased (Table 5.3). To fit the high emissions during the summer period, the decay rates of the all the soil humus pool were adjusted to increase CO_2 emissions from the decomposition of soil organic matter. The simulated average annual mineralization was around 160 kg N ha^{-1} changing these nutrient parameters. Carpenter-Boggs et al. (2000) also reported the mineralization amount from 150 to 160 kg N ha^{-1} during the growing season with 181 kg N ha^{-1} fertilization in South Dakota, US. The denitrification rate was reduced from 1.0×10^{-13} to 3.0×10^{-14}, similar to the calibrated values of Malone et al. (2014b), to reduce the N losses from denitrification. To properly initialize the soil microbial populations, Ma et al. (1998) suggested running the model for at least 10-12 years prior to the simulation period; accordingly, the model was run several times, and after each run initial residue levels were uploaded from the previous run to stabilize the organic matter pools. The stabilized initial nutrient concentrations are listed in Table 5.4.

5.2.4 Quantification of agronomic management effects using RZWQM

After calibrating and validating RZWQM2 with experimental data, annual GHG emissions were predicted based on the existing field conditions. Drawing on long-term historical weather data (1971—2000), alternative agronomic management practice scenarios supplementary to a corn-soybean (CS) rotation system were simulated with RZWQM over a 30-year period, to quantify their impacts on annual GHG emissions. Planting and harvest dates for simulated soybean [*Glycine max* (L.) Merr.] and corn were May 1st and November 1st, respectively. Each 'corn' year, N fertilization was applied prior to the planting date. Although split N application was performed at the experimental site, the fertilizer amount and application date for each year was decided by the farmer based on his experience (Crézé, 2015). The impact of splitting N application on GHG emissions over long-term period could be quantified by RZWQM2. In Canada, 19.8% of corn was cultivated with corn-soybean-wheat rotation system, and 18.7% was planted in corn-soybean rotation system to reduce the risk of soil erosion (Hamel and Dorff, 2015), improve soil quality and sustainability of agriculture (Karlen et al., 2006). However, the benefits of rotation cropping system for GHG emission mitigation have seldom been quantified. Therefore, the comparative agronomic management scenarios investigated were:

(i) Seventeen N fertilization rates from 0 to 300 kg ha^{-1} at 25 kg ha^{-1}'s interval in CS cropping system

(ii) Seven different N application dates: May 1st, May 11th, May 21st, May 31st, June 10th, June 20th, June 30th in CS cropping system.

(iii) Single N application and split-time applications totaling 200 kg N ha^{-1} (average N rates from 2013-2015) per year in CS cropping system

a. one before planting

b. one before planting, one after emergence

c. one before planting and one on June 15th, around two weeks before silking.

(iv) Two water table management scenarios in CS cropping system with 200 kg N ha^{-1} pre-plant applied

a. Free drainage (FD)

b. Controlled drainage with sub-irrigation (CD-SI). Water table depth maintained at 0.60 cm over the full growing season (May 1st to Oct 1st) with subirrigation applied from July 1st to Oct 1st at 20 mm per week.

(v) Corn-soybean rotation (CS) and continuous corn (CC).

5.2.5 N_2O emission factor (EF)

The N_2O emission factor (EF) was computed for simulating the impact of N fertilization rates on annual N_2O emissions following the method reported by Wang et al. (2016):

$$EF = \frac{N_2O_{AN} - N_2O_{ON}}{F} \qquad [5.1]$$

where EF is the N_2O emission factor induced by fertilizer; N_2O_{AN} is the direct N_2O emissions after N application (kg N ha^{-1} yr^{-1}), N_2O_{ON} is the direct N_2O emission without fertilizer, and F is the N fertilization rate (kg N ha^{-1} yr^{-1}). The EF was computed using the N_2O emission from only corn years in the corn-soybean rotation system to investigate the N fertilization impact on N_2O emission.

5.2.6 Model Accuracy Statistics

In this study, four statistics were used to evaluate the performance of RZWQM2 in simulating SWC, soil temperature, N_2O flux and CO_2 releases, relative to observed values: percent bias (PBIAS), root mean squared error (RMSE), index of agreement (IoA), and determination of coefficient (R^2) given as:

$$\mathrm{PBIAS} = \frac{\sum_{i=1}^{n}(O_i - P_i)100}{\sum_{i=1}^{n} O_i} \quad [5.2]$$

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(P_i - O_i)^2}{n}} \quad [5.3]$$

$$\mathrm{IoA} = 1 - \frac{\sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(|P_i - \bar{P}| + |O_i - \bar{O}|)^2} \quad [5.4]$$

$$R^2 = \frac{\sum_{i=1}^{n}(O_i - \bar{O})(P_i - \bar{P})}{\sqrt{\sum_{i=1}^{n}(O_i - \bar{O})^2 \sum_{i=1}^{n}(P_i - \bar{p})^2}} \quad [5.5]$$

where

n is the number of observations;

$\bar{O}$ is the mean observed value;

O_i is the i^{th} observed value;

$\bar{P}$ is the mean predicted (simulated) value; and

P_i is the i^{th} predicted value.

An IoA of 1 indicates perfect model accuracy and IoA > 0.7 a satisfactory model performance (Ma et al., 2012). PBIAS is a measure of the difference in mean simulated and observed values, for which a value of $\pm 15\%$ is considered satisfactory. The value of the R^2 is 1 when model estimates perfectly match observed data, and the model can be judged as satisfactory when $R^2>0.5$. However, these criteria should not be straightforward used for evaluating model performance in predicting daily N_2O and CO_2 emissions. Although these statistics are used to judge the performance of model simulations compared to field measurements of daily GHG emissions, they only indicate how well the model performs on a given day (Giltrap et al., 2010). Models may not perform satisfactorily in terms of RMSE and R^2 if the peak is not predicted on a given day such as leading or lagging behind the measured day, but the total amount of GHG emissions could still be reliable if the cumulative emissions are reasonably predicted, and the annual emissions for long term under different environmental conditions is the major concern in our study.

5.3 Results and discussion

5.3.1. Model evaluation

5.3.1.1. Soil temperature and soil water content (SWC)

The simulated and measured daily average soil temperature and soil water content are plotted in Figure 5.2 and Figure 5.3, respectively. Both simulated and observed soil water content are higher under CD-SI than FD in the validation year of 2014 and 2015 due to more water supply and water table control under CD-SI. Detailed statistics for RZWQM simulated soil water content and soil temperature at the soil depth of 6 cm under FD and CD-SI from 2012 to 2015 are listed in Table 5.5.

Given the greater water supply and water table management under CD-SI, both simulated and observed SWC of topsoil at 0.06 m depth were higher under CD-SI than under FD (Figure 5.3, Table 5.5). While little if any difference in observed soil temperature occurred between FD and CD-SI (Table 5.5; Figure 5.2), the simulated soil temperature was 5% higher under CD-SI than FD.

Based on the PBIAS, the SWC was over estimated by 11% under FD in the calibration phase, under-estimated by 5% under FD in the validation phase and overestimated by 1% under CD-SI in the validation phase, while for soil temperature the PBAIS values were 19%, 17% and 17% (Table 5.5). Overall, the simulated SWC followed the values and pattern of observed SWC data though it missed a few peaks. In contrast to SWC, the predicted soil temperature values were in closer agreement with observed data in terms of IoA and R^2. Although the average soil temperature was underestimated by around 18%, the trend of soil temperature was well simulated. The underestimation was mainly because the temperature was taken from soil samples at day time around noon, while the simulated soil temperature was predicted as an average on a daily basis. Some of the measured high values of soil temperature were close to the daily maximum air temperature, while the measured minimum air temperature at night could be very low. Generally, the performance of RZWQM2 in simulating the soil water content and soil temperature is satisfactory, with the IoA ranged from 0.80 to 0.96 and R^2 from 0.65 to 0.98 (Table 5.5).

5. 3.1.2. N_2O and CO_2 emissions

In the calibration phase, the model accuracy statistics (Table 5.6) and plots of simulated *vs*. observed daily N_2O and CO_2 emissions (Figures 5.4 and 5.5, respectively) showed the model performed well in simulating GHG emissions. However, it tended to underestimate some peaks. RZWQM2 over-estimated the total N_2O emissions under FD by 2% in the calibration phase. The average daily measured N_2O emission in 2012 was only 0.002 kg N ha^{-1} because the total N fertilization was 70 kg ha^{-1}, and RZWQM2 correctly simulated low N_2O emissions accordingly. The model satisfactorily predicted the CO_2 emissions with the PBIAS within 3%, and both IoA and R^2 were higher than 0.70 in the calibration phase.

In the validation years, RZWQM2 simulated average daily N_2O emissions under FD (0.0115 kg N ha^{-1}) with PBIAS=13%, IoA = 0.71, and R^2 =0.56, showing a good performance in predicting the daily N_2O emissions under FD in 2014 and 2015. However, the average daily measured N_2O emissions under CD-SI were 0.0137 kg N ha^{-1}, compared to the simulated value of 0.120 kg N ha^{-1}, indicating a 13% underestimation of N_2O emission. The IoA was only 0.21 and R^2 was 0.16 because RZWQM2 failed to catch the peak of daily N_2O emission 20 days after fertilization under CD-SI on June 27th, 2014 (0.35 kg N ha^{-1}), which was almost 58% over the 45 measurements within the two years. The PBIAS would be 75%, while both IoA and R^2 could be 0.87 if the peak was removed. This peak flux occurred shortly after a heavy rainfall event (5.4 cm) on June 25th, however, it was only observed in CD-SI, while in FD the measured N_2O emission was 0.07 kg N ha^{-1}. The measured SWC in FD and CD-SI on that day was 0.32 and 0.41, respectively, which indicated a more anaerobic environment and higher denitrification rate in CD-SI than FD. However, the simulated SWC were 0.31 and 0.33 for FD and CD-SI. In addition, the measured soil temperature was 29°C on that day, while the RZWQM simulated temperature was only 19°C. The failure to predicte the SWC after heavy rainfall under CD-SI and the under-estimation of soil temperature resulted in missing N_2O flux peaks. Since the N_2O emission on June 26th is unknown, we suggest that N_2O emissions be measured more frequently after rainfall . Although the statistics for daily N_2O emission prediction was not satisfactory for CD-SI, the model still successfully predicted higher N_2O emissions and lower CO_2 under CD-SI as compared to FD. In addition, the model performance was better than similar studies using other models, such as DNDC with PBIAS from -41% to 221%, DAYCENT with PBIAS from -32% to +188% under different N treatments in Quebec (Smith et al., 2008b).

CO_2 emissions were over-estimated by 7% in FD, but under-estimated by 9% in CD-SI. The average measured CO_2 emissions were 18.2 kg ha^{-1} and 19.5 kg ha^{-1}, while simulated values were 20.7 kg ha^{-1} and 16.1 kg ha^{-1} in FD and CD-SI, respectively. Both simulated and measured values indicated higher CO_2 emissions under FD. Linn and Doran (1984) reported that the CO_2 production reached a peak value at 60% WFPS (water filled pore space). In this study, the simulated average WFPS was 65% and 75% WFPS in FD and CD-SI. The higher soil water resulted in less O_2 availably for aerobic microbial activities and lower CO_2 emissions in CD-SI.

5.3.2. Simulating long term impacts of different N rates on annual GHG emissions

Long term simulations using historical weather data from 1971 to 2000 served to investigate the impact of different N application rates and split N fertilizer applications on GHG emissions. Within the validated RZWQM2 model, pre-seeding nitrogen fertilizer applications at 13 different rates, ranging from 0 to 300 kg ha^{-1} in intervals of 25 kg ha^{-1}, were applied at the beginning of each season under corn-soybean rotation systems, and the resulting GHG emissions were simulated. A plot of mean annual GHG emissions *vs.* N fertilization rate (Figure 5.6a), shows that the RZWQM simulated annual N_2O emissions in the rotation's corn years which increased linearly from 1.47 kg N ha^{-1} to 3.80 kg N ha^{-1} as N fertilization application rate increased from 0 to 300 kg N ha^{-1}.

The annual N_2O emission in corn planting years can be computed using the N application: $E = 0.0088F+1.1955$, R^2=0.981 (Figure 5.6a), Where E is the N_2O emissions, and F is the quantity of N fertilizer applied per year (kg N ha^{-1} y^{-1}). The predicted results are consistent with the results of experiments reported by Bouwman (1996), who developed a linear equation linking annual N_2O emissions to N fertilization rate based on field experiments: E= 1.25F+1. Similar results were reported by Roelandt et al. (2005).

At fertilization rates exceeding 150 kg N ha^{-1}, RZWQM2 simulated N_2O emissions equivalent to 1.23% to 1.56% of the added fertilizer N, a level consistent with the findings of MacKenzie et al. (1998), who reported a linear increase of N_2O emissions with increasing N fertilization rate, and found the quantity of N released as N_2O to represent 1.0% to 1.6% of the N applied as fertilizer. Moreover, Helgason et al. (2005) summarized the data sets from 400 sites across Canada over several decades and estimated a linear coefficient of N_2O emissions to fertilizer N which accounted for 1.18% of N applications. The EFs ranged from 0.52% to 0.76% (Figure 5.6b) within the range from 0.003 to 0.03 suggested by IPCC (2016), who set the default value for mineral fertilized soil EF at 0.01. Similar to the findings from Wang et al. (2016), the simulated EF value increased linearly when N application increased from 100 kg ha^{-1} to 300 kg ha^{-1}, and showed negligible difference when added N was within 100 kg ha^{-1}.

In contrast to N_2O emissions, CO_2 emissions responded differently to incrementally greater N fertilizer application rates, which increased when fertilizer rates increasing from 0 to 100 kg N ha^{-1} because of higher accumulated crop residues, but decreased slowly from 3.88 to 3.80 Mg CO_2 ha^{-1} as the N fertilization rate rose from 100 to 300 kg N ha^{-1} (Figure 5.6a). Similar findings of decreasing CO_2 emissions with higher N applications were reported by Al-Kaisi et al. (2008), Kowalenko et al. (1978), and Ma et al. (1999) due to lower soil pH from nitrification and reduced microbial activities, while Dick (1992) argued that the microbial activities might be stimulated with increasing N fertilization as more plant biomass returned to soil profile. RZWQM2 did not compute the changing soil pH value corresponding to nitrification, so the predicted decreasing CO_2 emission with increasing N fertilization could be explained by the depletion of O_2 from the soil through the enhanced nitrification process in the soil. Consequently, the predicted CO_2 emission from aerobic microbial respiration was reduced when more soil O_2 was consumed by nitrification with elevating N input. In addition, the CO_2 also acted as a carbon source for the nitrification process, as simulated by RZWQM2.

The simulated corn yield increase linearly with N application rate increased from 0 to 100 kg N ha^{-1}, then it showed a declining positive response up when fertilization rate was between 100 to 250 kg N ha^{-1} before levelling off when N rate was above 250 kg N ha^{-1} (Figure 5.7). Cambouris et al (2016) observed maximum corn yield between 150 to 250 kg N ha^{-1} in four different sites in Quebec, depending on the soil texture. They determined the NUE (nitrogen use efficiency) as: (Total N uptake-Total N uptake at 20 kg N which is the starter application amount) / Total N applied. The NUE decreased from 59% to 42% when N application increased from 100 kg N ha^{-1} to 250 kg N ha^{-1}. They proposed N fertilizer amounts ranging from 100 to 150 kg N ha^{-1} to optimize corn yield and quality. In our simulation, we defined the starter fertilization rate at 25 kg N ha^{-1} to compute the NUE. Our simulated NUE showed comparable results with Cambouris et al (2016). It responded positively with increasing fertilization from 25 kg N ha^{-1}, and reached to the maximum rate at 66% when N was applied at 125 kg N ha^{-1}, then the NUE decreased with rising fertilization rate (Figure 5.7). The average corn grain yields of 2016 in Quebec was reported at 10.14 Mg ha^{-1} (Institut de la statistique du Québec, 2016) and in Montérégie region was 10.94 Mg ha^{-1}, which were achieved at the fertilization rate of 100 and 125 kg N ha^{-1}, respectively as predicted by RZWQM2. The maximum NUE was estimated with fertilization rate of 125 kg N ha^{-1}, and the grain yield was 11.25 Mg ha^{-1} accordingly. Predicted corn yield and GHG emissions suggested that the minimum N application N should be higher than 100 kg ha^{-1} to maintain the average yield of 10 Mg ha^{-1}, but to obtain the highest efficieny of N uptake by corn, 125 kg N ha^{-1} is required. Although maximum yield was obtained at N fertilization rate of 300 kg ha^{-1}, the NUE was only 46% and the annual N_2O emission was 3.80 kg N ha^{-1}. Therefore, the optimal N application rate ranging from 125 to 175 kg N ha^{-1} is suggested in order to maintain a high yield (11.25-12.18 Mg ha^{-1}) yet minimize annual N_2O emissions (2.16-2.55 kg N ha^{-1}). It should be noted that the suggested N application rates and NUE were only based on the corn-soybean rotation system. The soybean yield was not affected by the rate of fertilizer application in corn planting years.

Singh (2013) used another definition for NUE computation as grain yield/ N applied for the field experiment from 2008 to 2009 at the same site (St Emmanuel), indicating that NUE decreased with increasing N application, due to more N loss from leaching and dentrification (Liang et al., 1991; Mejia and Madramootooo, 1998). We computed NUE using this method and found it to be constistent with Singh (2013). The simulated NUE was 90 kg kg^{-1} and 51 kg kg^{-1} with fertilization amount of 125 kg N ha^{-1} and 250 kg N ha^{-1}, respectively, which was comparable to the values computed from the field experiment reported by Singh et al. (2013), with the NUE at 41 kg kg^{-1} at high N (250 kg N ha^{-1}) application and 99 kg kg^{-1} at low N (130 N kg ha^{-1}) application. This comparison showed the reliabilty of RZWQM2 for simulating the N impacts on corn yield at this site.

5.3.3. N fertilization timing and split application

The N_2O and CO_2 emissions were predicted under one-time N application on seven different days: May 1st, May 11th, May 21st, May 31st, June 10th, June 20th and June 30th (Figure 5.8). The simulated results suggested that later N application resulted in N_2O and CO_2 emission reduction. The RZWQM2 predicted up to 13.6% less N_2O and 3.9% less CO_2 emission when the N fertilization was applied on June 30th compared to May 1st. Surplus N has potential to cause environmental problems due to the N loss through leaching or atmosphere because of different crop N demand at different growing stages (Wang et al., 2016). The RZWQM2 simulated N_2O emissions were affected by the timing of N application because 63% of the total N uptake by crops was from June to July (Figure 5.9). Later application of N fertilizer resulted in less nitrification and denitrification, due to less soil NH_4^+ and NO_3^- concentration after crop N uptake. Early one-time N application led to a longer nitrification period and more N_2O was released before the N was taken up by the crop. However, corn yield was reduced by 0.1% to 5.4% due to the N stress in the early crop growing period when N fertilization was applied late. CO_2 emission was less affected by the N fertilization timing since the crop growth was only slightly reduced. Results from long-term RZWQM2 simulations indicated that splitting the fertilization based on the crop N need could be a strategy for reducing N_2O emissions while maintaining crop yield.

Although fertilization on June 30th, around silking, has the greatest potential to reduce the N_2O and CO_2 emissions compared to other days, it should be noted that later N fertilization could be inappropriate once the corn reaches a certain height. Therefore, it is more reasonable to apply the N fertilizer two weeks before silking when the field is still trafficable by machinery. Long term simulations suggested that N application split between pre-plant and postemergence had a negligeable impact on GHG emissions (0.26% reduction for N_2O and 0.31% for CO_2), whereas N application split between pre-plant and two weeks before silking resulted in substantial reductions in N_2O and CO_2 emissions (11.0% and 0.33%, respectively), without reducing crop yield. This indicates that the timing of the second N application has a substantial influence on GHG emissions compared to a single application. Laboratory results by Fernández et al. (2016) also suggested that splitting N applications in a tile-drained field was an effective strategy to reduce N_2O emissions by 18% as compared to a single application (1.62 vs 1.32 kg N ha^{-1}), while not affecting corn grain yield. Both our simulated results and the measured values from Fernández et al. (2016) indicated the potential of splitting N to reduce N_2O emissions in sub-surfaced drained fields. It should be noted that the extra application of fertilizer would require 1.4 L to 1.8 L diesel per hectare by the tractors for field operations (Hanna, 2001; Grisso et al., 2010), which results in 3.78 to 4.86 kg ha^{-1} more CO_2 emissions and 0.0003 to 0.0004 kg N ha^{-1} more N_2O emissions from fossil fuel. Therefore, splitting N fertilization at pre-plant and two weeks before silking is still recommended, which reduces N_2O emission by 0.3 kg N ha^{-1} and CO_2 emission by 12.67 kg ha^{-1}.

5.3.4. Controlled drainage with sub-irrigation impact on GHG emission

The CD-SI was applied over the full growing season (May 1st to Oct 1st) to simulate GHG emissions under water table management, and these emissions were compared to those under free drainage conditions. Long-term simulated results showed that CD-SI improved the corn and soybean yields by 8% and 3% compared to FD. The simulated results showed very similar trend with historical records at the same site. Corn yield benifit from CD-SI by 3-7% at the St Emmanuel site from 1993 to 1996 (Zhou et al. 2000; Mejia et al. 2000), while in 2001 and 2002 the corn yield was 32.9% to 36.2% higher in CD-SI than FD, due to extremely dry conditions during both growing seasons (Stampfli and Madramootoo, 2006).

The long-term simulation indicated that annual N_2O and CO_2 emissions under CD-SI were respectively 21% higher and 6% lower than under FD in corn-soybean (CS) rotation cropping system (Table 5.7). The CD-SI resulted in higher SWC and less O_2 in the soil during the growing season, which led to more denitrification and higher N_2O emissions. The RZWQM2 simulated long-term average WFPS for the 0-0.05 m soil layer, during the growing season (July 1st to September 30th) was 48% and 68% for the FD and CD-SI treatments, and 62% and 78% at for the 0-0.5 m soil layer. A higher WPFS resulted in greater denitrification (19.89 kg N ha^{-1}) and associated N_2O emissions (2.76 kg N ha^{-1}) under CD-SI, than under FD (11.17 kg N ha^{-1} denitrification and 2.27 kg N ha^{-1} N_2O emissions). Weier et al. (1993) similarly measured an increase in N losses from denitrification with an increase in WFPS. However, they found no significant difference in N_2O emissions arising from nitrification between different water table management treatments, though nitrification under FD and CD-SI generated 62% and 52% of simulated N_2O, respectively. Bateman and Baggs (2005) indicated that the proportion of N_2O emission from denitrification and nitrification were determined by the WFPS: at a WFPS of 70% all N_2O emissions were from denitrification, while at a WFPS between 35% and 60% most N_2O was produced by nitrification (81% N_2O emitted from nitrification at 60% WFPS).

In our study, in contrast to N_2O emissions, simulated CO_2 emissions were less affected by the imposition of CD-SI (*vs* FD). The CD-SI regime reduced CO_2 emissions by 6% as the soil profile's SWC was higher and its O_2 availability less. This finding is consistent with other field studies with different water table management regimes (Edwards, 2014; Grant, 2014), which found CO_2 emissions to be mainly affected by soil temperature, and to a much lesser extent by SWC.

5.3.4. Corn-soybean rotation

The long-term simulation indicated that the corn-soybean rotation (CS) system was found to reduce both CO_2 and N_2O emissions by 18.8% and 20.7%, respectively, compared with continuous corn (CC) (Figure 5.10a). The reduction of annual N_2O emission was due to less N application amount under rotation system, while less crop residue from the CC cropping system resulted in less CO_2 emission because corn produced much more biomass than soybean. The RZWQM2 simulated 55.8% more above ground biomass and 51.8% more below ground biomass under the CS than the CC cropping system (Figure 5.10b). The results are supported by the experiments reported by Campbell al et al. (2014) with significantly greater N_2O and CO_2 emission under a CC system than a CS system in Wooster and Hoytville, Ohio. Vyn et al. (2006) also reported a 14% higher CO_2 emission under a CC cropping system compared to a CS cropping system due to the greater corn residue returned to the soil.

5.4 Conclusions

The performance of RZWQM2 in predicting N_2O and CO_2 emissions was evaluated under different water table management practices. The RZWQM2 model was calibrated and validated based on 2012 to 2015 soil temperature, soil water content, N_2O and CO_2 emission data from a subsurface-drained field in Southern Quebec. The SWC and soil temperature were well simulated, and different years' predicted cumulative growing season GHG emissions were in close agreement with the measured values. Trends in N_2O and CO_2 emissions were also comparable to trends in measured values, though some peaks were missed.

After model calibration and validation, different fertilization timing and water table management practices were implemented to investigate the impact of N fertilization rate and water table management practices on GHG emissions. The long-term average annual N_2O and CO_2 emissions would be 2.16-2.55 kg N ha^{-1} and 3854-3887 kg ha^{-1} with 125-175 kg N ha^{-1} of dry urea fertilization under free drainage and corn-soybean rotation cropping system. The RZWQM2 output suggested that N_2O emissions would respond linearly to an increasing N fertilization rate, while CO_2 emissions would increase with a rising N application rate with higher corn residue but decrease slightly when N fertilization gets higher than 100 kg N ha^{-1} and less soil O_2 was available. Higher N fertilization rates were found to promote corn production and exacerbate N_2O emissions. To optimize the corn yield and NUE, yet minimize GHG emissions, a N fertilization rate of 125-175 kg N ha^{-1} was suggested. The timing of N application could affect the N_2O emission because the crop N demand differred with the growing stage. Splitting the N fertilizer application had the potential to reduce the N_2O emissions by 11% but had very limited effects on CO_2 emissions. On average, CO_2 emissions were reduced by 6% and N_2O emissions increased by 21% under CD-SI compared to FD, as a result of the higher SWC and lower O_2 availability of the soil under CD-SI. The corn-soybean rotation system significantly decreased both N_2O and CO_2 emissions by 20.7% and 18.8% due to less N fertilizer requirement and less crop residue accumulated. The RZWQM2 model proved to be a promising tool in simulating the GHG emissions under different agronomic management scenarios.

Acknowledgement

We thank Agriculture and Agri-Food Canada for their financial support, in the form of a research contract to Professor Madramootoo, for the collection of the field data and greenhouse gas measurements. We appreciate the hard work of students of Dr. Madamootoo's lab, who collected the four years' field data. We gratefully acknowledge Hicham Benslim, Blake Bissonnette and Hélène Lalande for their technical and analytical assistance. We thank the landowner, Mr. Guy Vincent and his family, who allowed us to conduct this experiment on their farm. Finally, we thank Dr. George Dodds for proof reading the article.

Table 5.1. Crop, nitrogen fertilizer application dates and rates (kg N ha^{-1}), and modelling use of GHG and other data measured in field study.

Crop	Year	Type of drainage	*N fertilizer application (kg ha^{-1})				
			Seeding		Sidedressing		Overall
			Date	Rate	Date	Rate	Rate
Yellow bean	2012	FD	21-June	60	20-Aug	10	70
Corn	2013	FD	1-May	44	29-May	115	159
Corn	2014	FD and CD-SI	11-May	44	7-Jun	160	204
Corn	2015	FD and CD-SI	2-May	28	29-May	200	228

*Fertilizer was dry and granular urea; broadcast and then incorporated using a row crop cultivator. FD, free drainage; CD-SI: controlled drainage with subirrigation.

Table 5.2. Calibrated RZWQM2 soil hydraulic parameters.

Layer	Depth	ρ	Soil Water Retention				Lateral	Vertical
	(m)	(Mg m^{-3})	θ_s (m^3m^{-3})	θ_r (m^3m^{-3})	τb (mm)	λ	k_{sat} (mm h^{-1})	k_{sat} (mm h^{-1})
1	0-0.05	1.36	0.487	0.025	-14.5	0.254	8	20
2	0.05-0.25	1.60	0.396	0.025	-24.1	0.231	35	70
3	0.25-0.45	1.46	0.449	0.025	-5.9	0.082	17	35
4	0.45-0.80	1.40	0.472	0.025	-3.9	0.072	20	40
5	0.80-1.20	1.40	0.464	0.025	-3.8	0.083	20	40
6	1.20-1.50	1.40	0.464	0.025	-3.5	0.087	20	40
7	1.50-2.00	1.40	0.464	0.075	-3.0	0.170	0.1	0.1

[a] ρ = bulk density, θ_s = saturated soil water content, θ_r = residual soil water content, τb = bubbling pressure, λ = pore size distribution index, k_{sat}=saturated hydraulic conductivity.

[b] Other required parameters include A1 (set to zero), B (computed using the RZWQM default constraint) for all layers, N_1 (set to zero), and K_2 and N_2 (computed using the RZWQM default constraints) for all layers (Ahuja et al., 2000b). The lateral hydraulic gradient was adjusted to a value of 1.5×10^{-6}.

Table 5.3. Calibrated RZWQM2 non-default hydrology and nutrient parameters.

Parameters	Value	Default
Hydrology component		
Albedo of crop	0.55	0.7
Drain depth (m)	1.00	-
Drain spacing (m)	15.0	-
Radius of drain (m)	7.6	-
Surface soil resistance for S-W	150	37
Nutrient component		
Nitrification	8.5×10^{-10}	1×10^{-9}
Decay rate of slow residue pool	1.673×10^{-8}	1.673×10^{-7}
Decay rate of fast residue pool	5.14×10^{-8}	8.14×10^{-6}
Decay rate of fast soil humus pool	5.5×10^{-7}	2.5×10^{-7}
Decay rate of intermediate soil humus pool	5×10^{-7}	5×10^{-8}
Decay rate of slow soil humus pool	4.7×10^{-9}	4.5×10^{-10}
Denitrification rate	3.0×10^{-14}	1.0×10^{-13}

Table 5.4. Initial concentrations for organic matter pools

Layer	Carbon pool					Microbial population (organisms g^{-1} soil)		
	Residues (μg C g^{-1})		Humus (μg C g^{-1})					
	Slow	Fast	Fast	Intermediate	Slow	Aerobic heterotrophs	Autotrophs	Anaerobic heterotrophs
1	122	1759	50	28	2121	3640000	17000	6366
2	195	440	29	19	8473	724867	9082	8356
3	281	547	32	29	12000	759544	7269	15000
4	282	534	14	12	9160	259766	2943	14000
5	0	1	278	148	12000	19000	1530	2278
6	0	0	405	217	12000	17000	1220	2222
7	111	170	0	0	277	2370	76	733

Table 5.5. Statistics for RZWQM2 simulated soil water content (SWC) and soil temperature at 6 cm soil profile under FD and CD-SI from 2012 to 2015. The units of average and RMSE for SWC and soil temperature are cm^3 cm^{-3} and ºC, respectively. Obs_{avg}: the average of observed values; Sim_{avg}: the average of simulated values.

		Obs_{avg}	Sim_{avg}	PBIAS	RMSE	IoA	R^2
2012-2013	SWC	0.28	0.29	-7%	0.06	0.96	0.92
FD	Soil T	17.3	14.0	19%	3.63	0.96	0.98
2014-2015	SWC	0.27	0.26	5%	0.06	0.80	0.65
FD	Soil T	18.3	15.1	17%	4.57	0.81	0.83
2014-2015	SWC	0.29	0.30	-1%	0.04	0.92	0.85
CDSI	Soil T	18.4	15.9	17%	4.65	0.80	0.82

Table 5.6. Statistics for RZWQM2 simulated N_2O and CO_2 emissions from soil profile under FD and CD-SI from 2012 to 2015. The units of average and RMSE for N_2O and CO_2 are kg N ha^{-1} and kg ha^{-1}, respectively.

		Obs_{avg}	Sim_{avg}	PBIAS	RMSE	IoA	R^2
2012-2013	N_2O	0.0110	0.0113	-2%	0.02	0.68	0.50
FD	CO_2	11.88	12.27	-3%	6.73	0.80	0.71
2014-2015	N_2O	0.0102	0.0115	-13%	0.02	0.71	0.56
FD	CO_2	18.18	19.54	-7%	10.18	0.76	0.62
2014-2015	N_2O	0.0137	0.0120	13%	0.053	0.21	0.16
CDSI	CO_2	17.83	16.14	9%	9.92	0.74	0.63

Table 5.7. Annual RZWQM2 output under different water table treatments

Treatment	**N_2O** kg N ha^{-1}	**CO_2** Mg ha^{-1}	**Mineralization** kg N ha^{-1}	**Denitrification** kg N ha^{-1}	**Drainage** **(m)**
FD	2.27	4.11	163.89	11.17	0.350
CD-SI	2.76	3.87	127.61	19.82	0.479
	21%	-6%	-22%	77%	37%

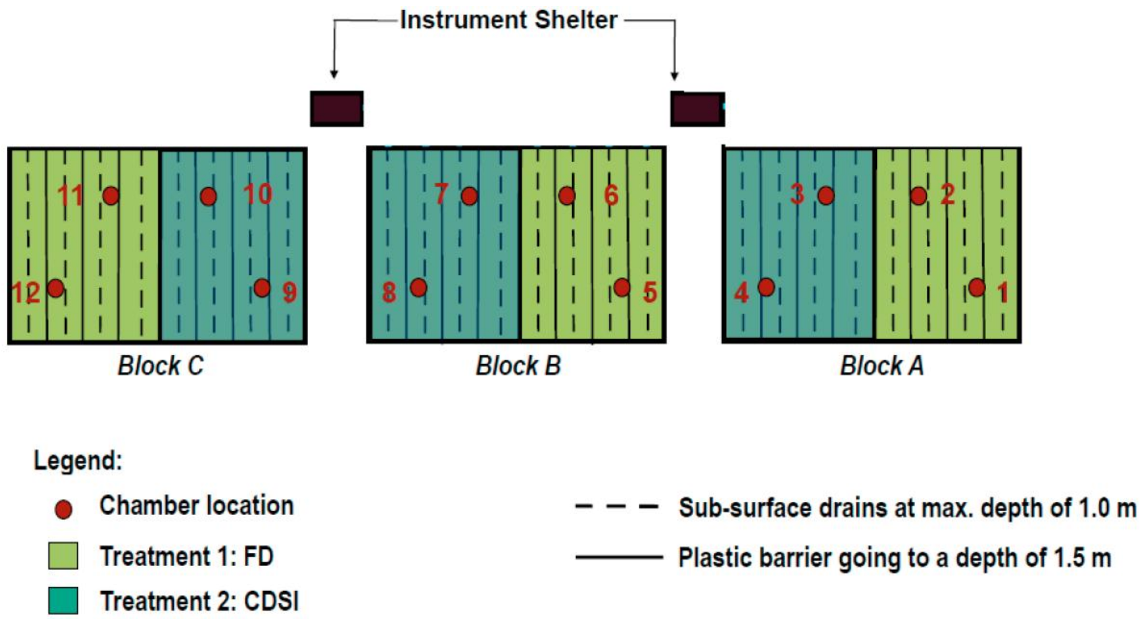

Figure 5.1*. Experimental layout of field study in 2014 and 2015. In 2012 and 2013 all plots were under free drainage (adapted from Crézé, 2015).*

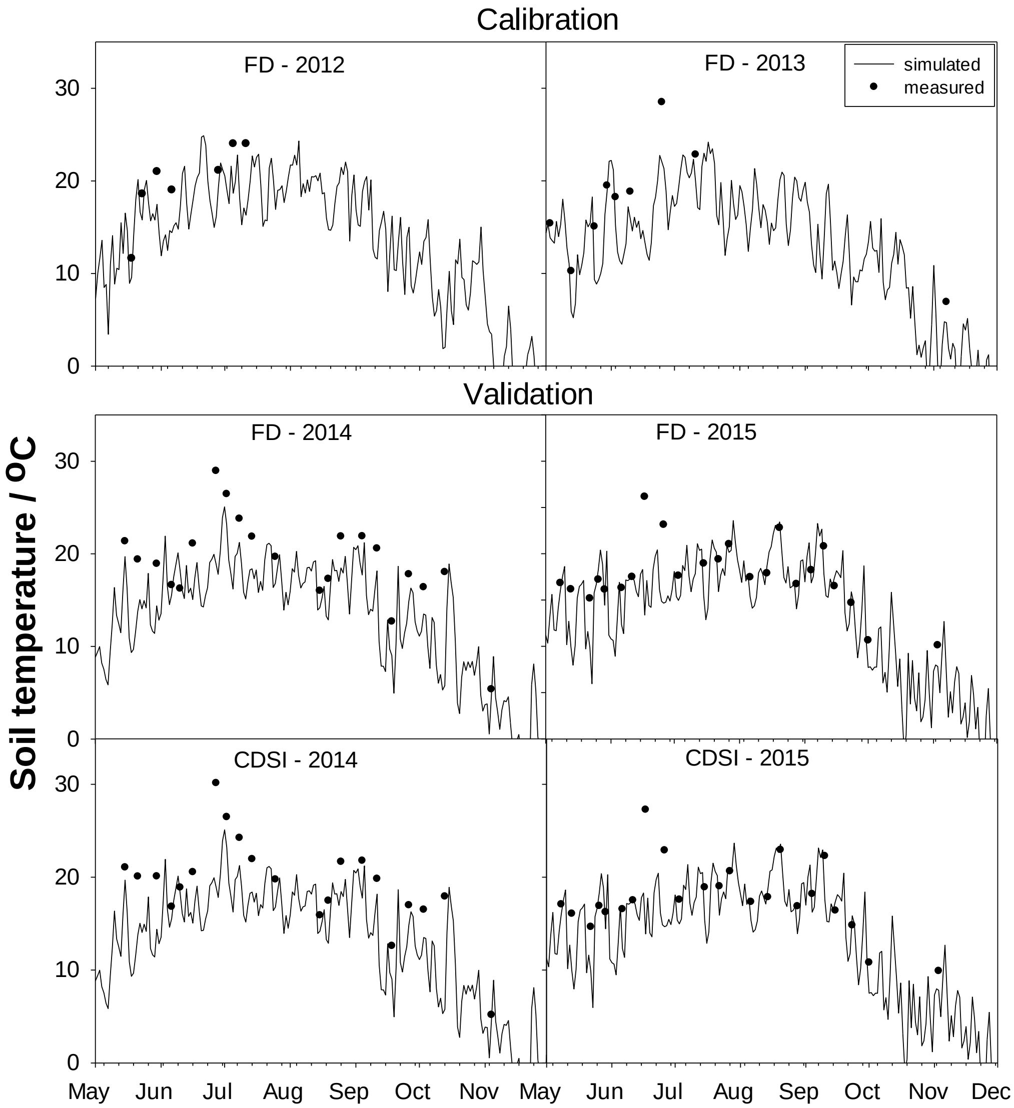

Figure 5.2. *Comparisons between RZWQM2 simulated and observed soil temperature under FD and CD-SI in calibration and validation phases from 2012 to 2015.*

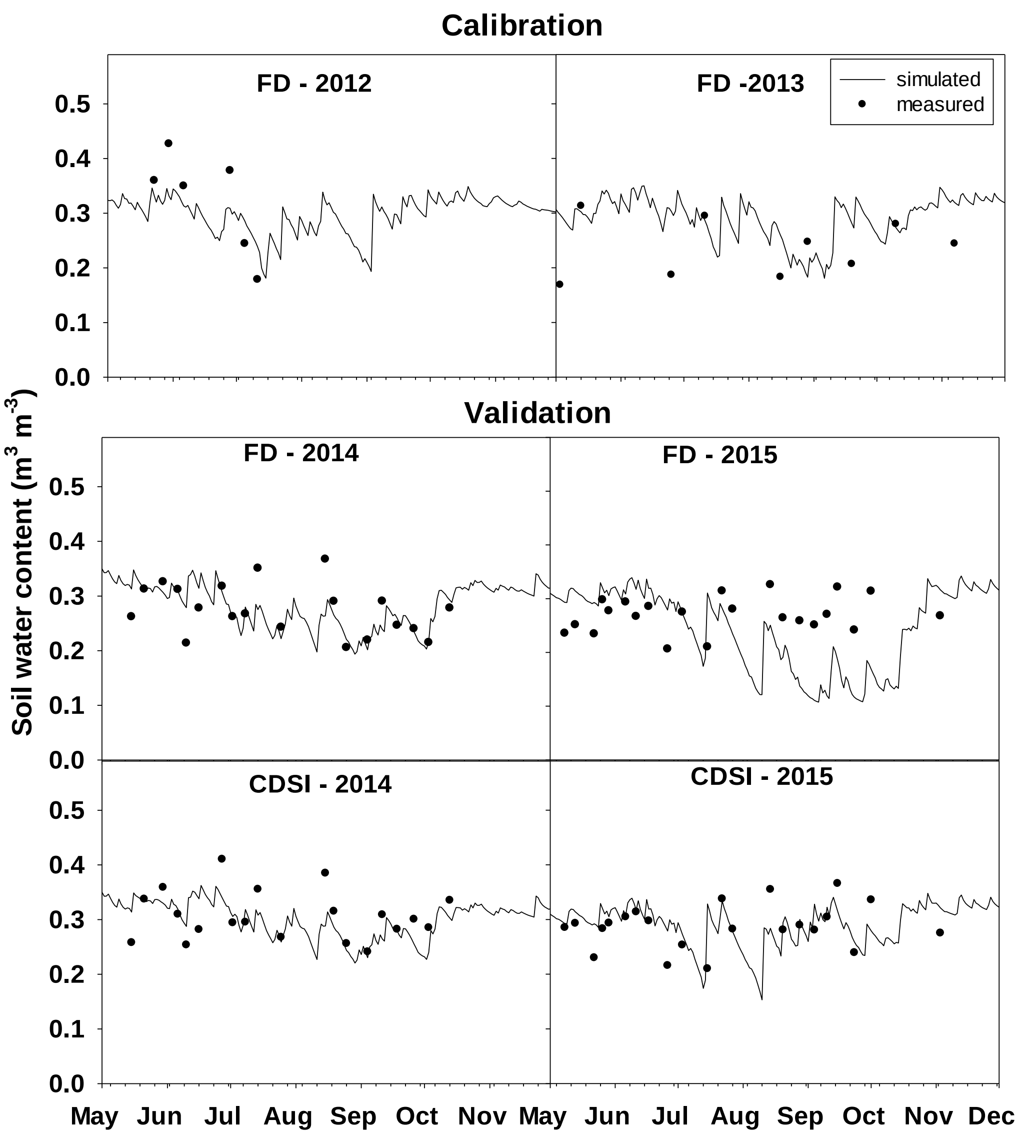

Figure 5.3. *Comparisons between RZWQM2 simulated and observed soil water in calibration and validation phases, under FD and CD-SI from 2012 to 2015.*

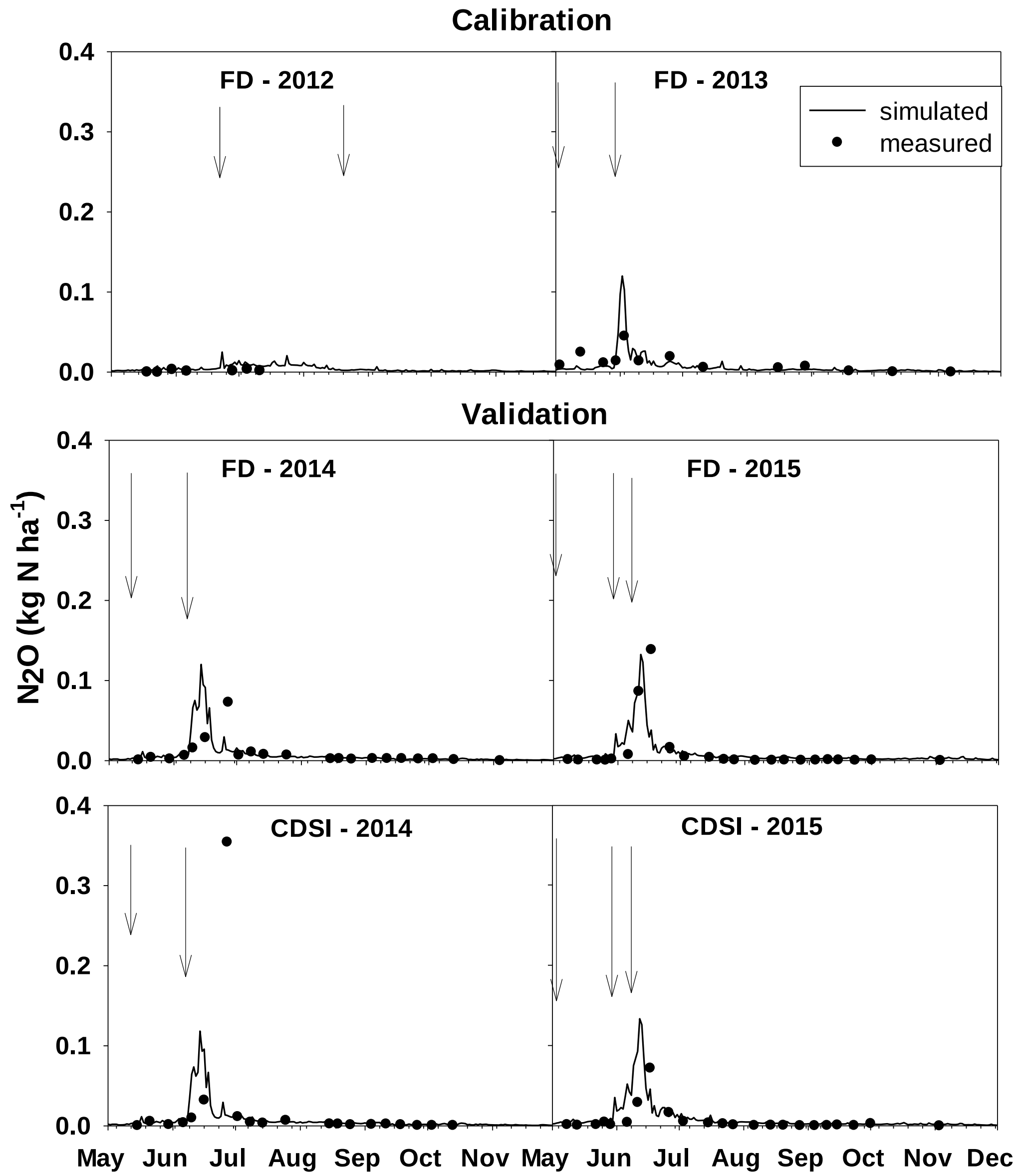

Figure 5.4. *Comparisons between RZWQM2 simulated and observed N_2O emissions in calibration and validation phases under FD and CD-SI from 2012 to 2015. Arrows are fertilizer application.*

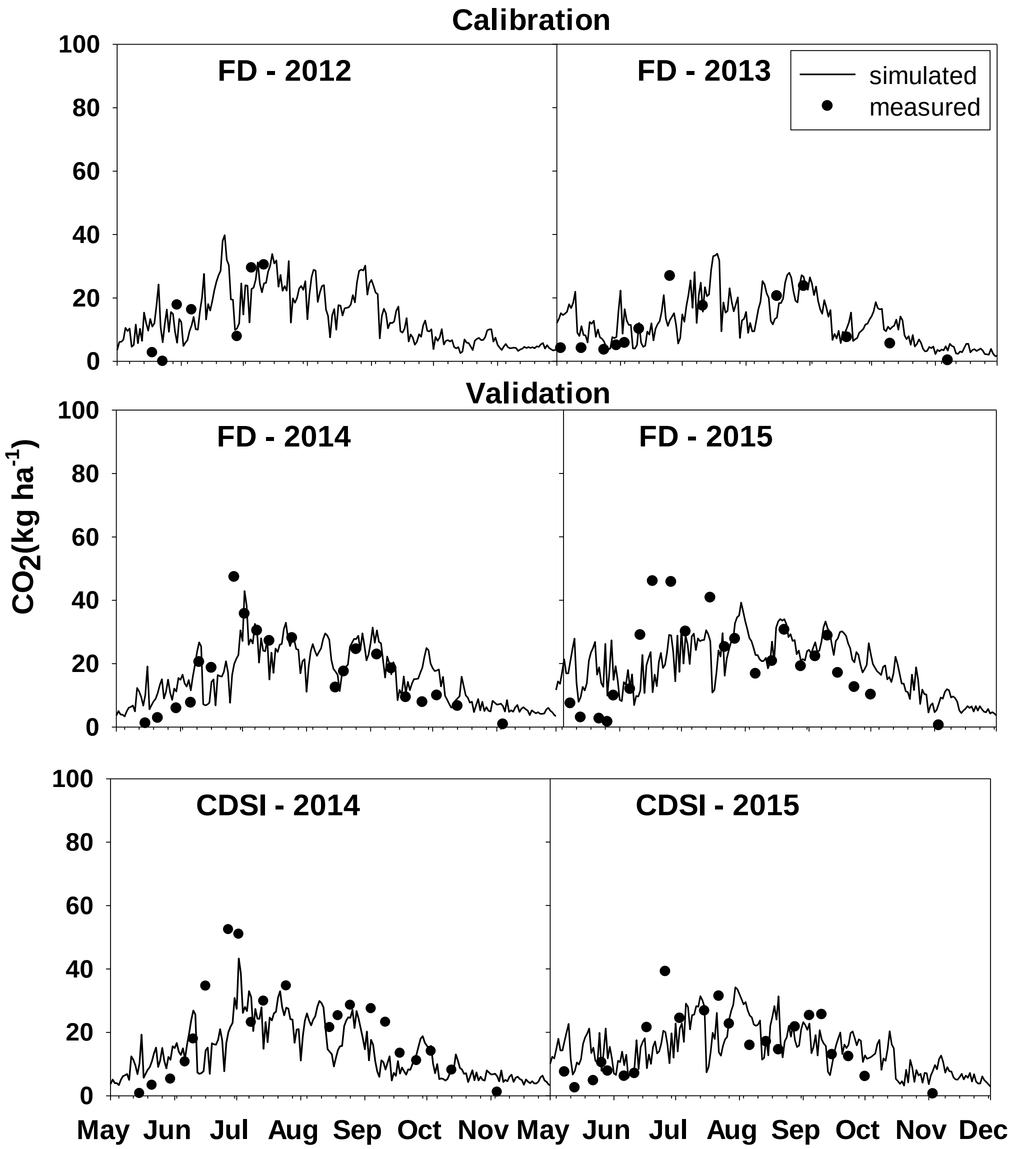

Figure 5.5. *Comparisons between RZWQM2 simulated and observed CO_2 emissions in calibration and validation phases under FD and CD-SI from 2012 to 2015*

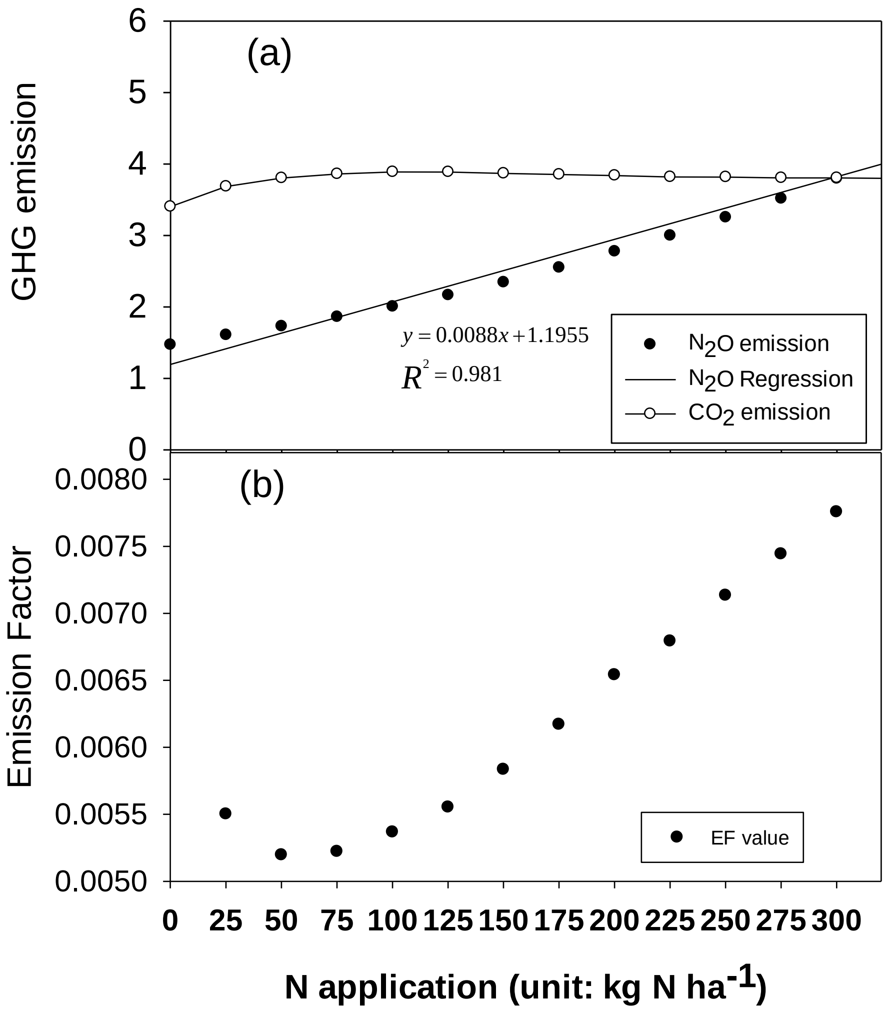

Figure 5.6. *(a) Simulated long-term annual GHG emissions (N_2O: kg N ha^{-1}; CO_2: Mg ha^{-1}) and (b) N_2O emission factors for corn years in the corn-soybean rotation system under different N rates.*

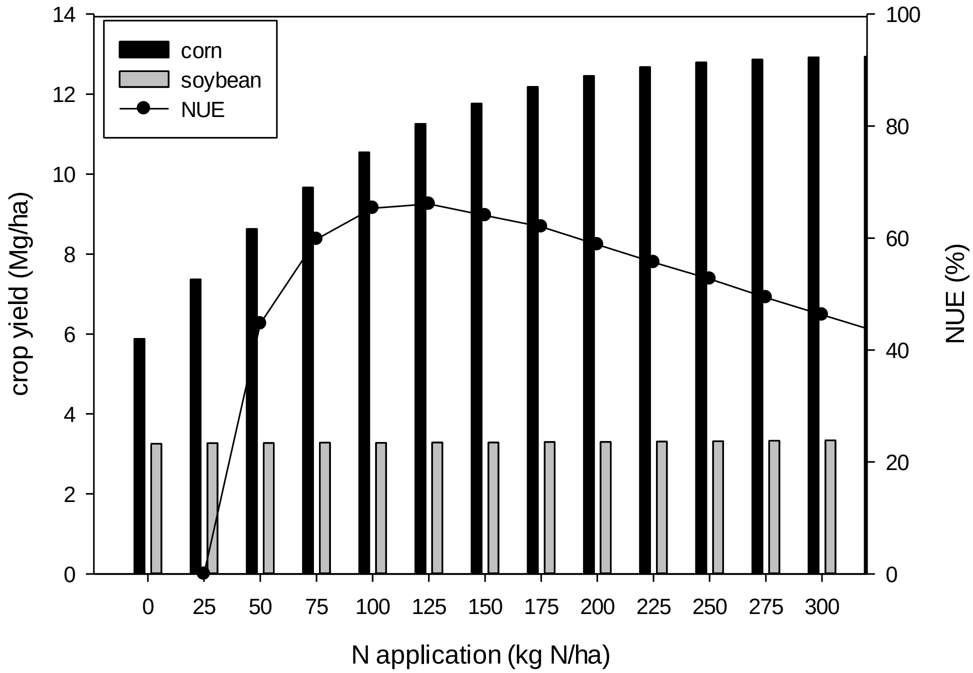

***Figure 5.7**. Corn and soybean yield (Mg ha^{-1}) and nitrogen use efficiency [NUE%, method by Cambouris et al (2016)] responses to different N application rates*

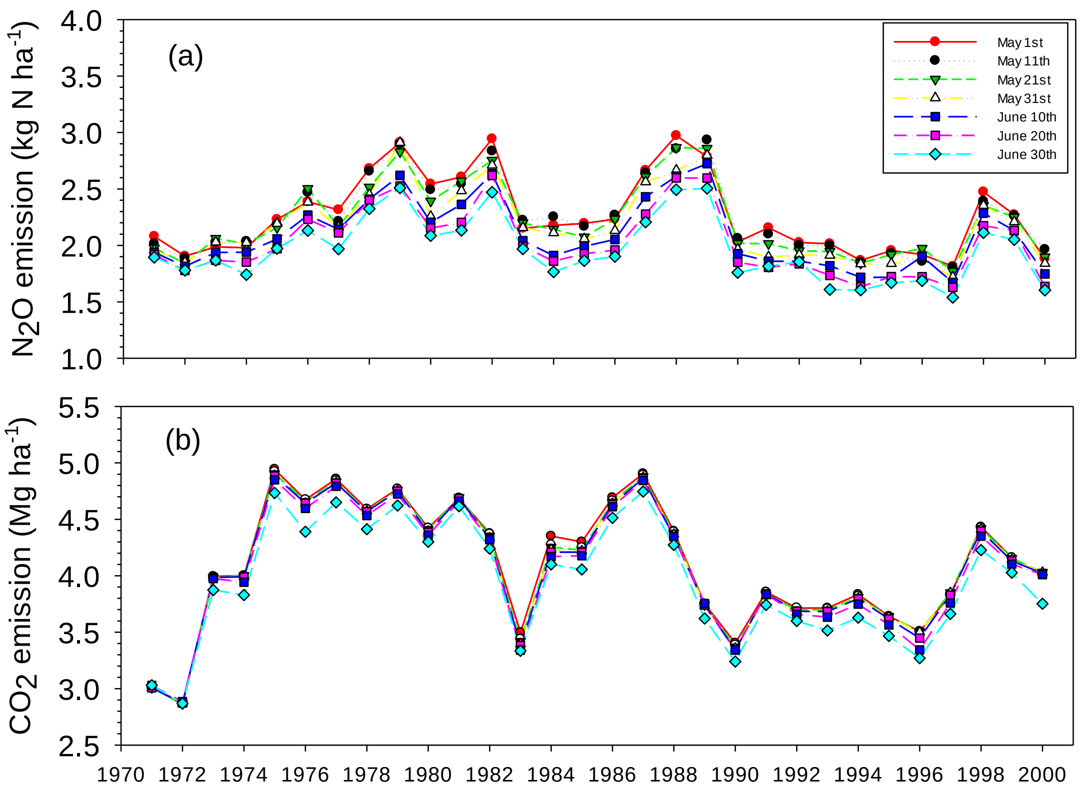

***Figure 5.8**. Long term simulated yearly N_2O (a) and CO_2 emissions under different fertilization days*

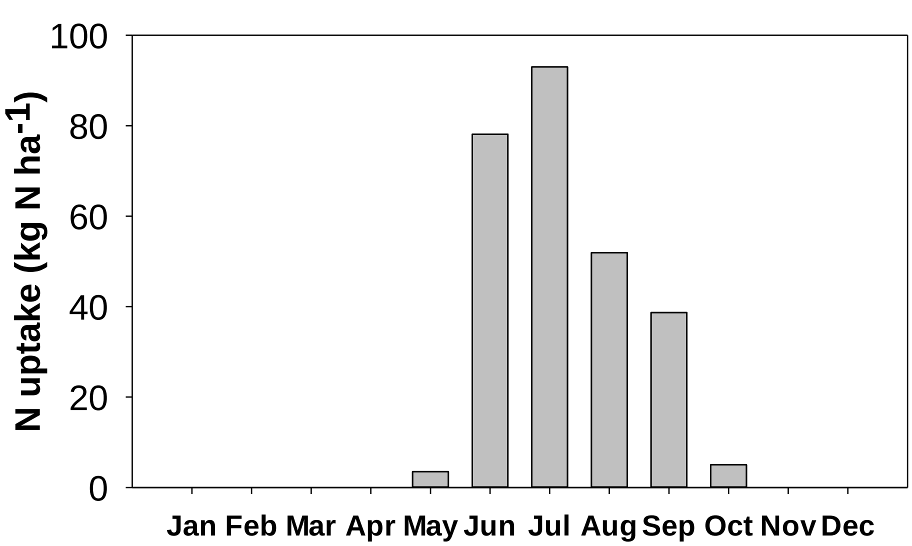

***Figure 5.9**. The RZWQM2 simulated long-term average monthly N uptake by corn*

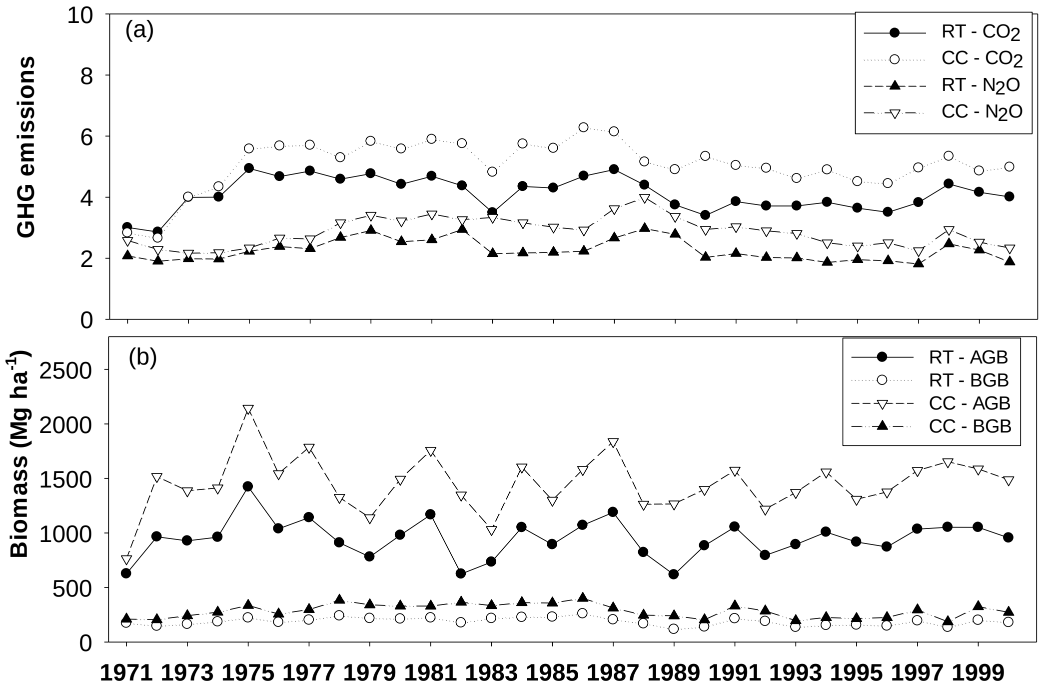

Figure 5.10*. The GHG emission, AGB (above ground biomass) and BGB (below ground biomass) under rotation (RT) and continuous corn (CC) cropping system. Units: CO_2: Mg ha^{-1}; N_2O: kg N ha^{-1}; AGB: Mg ha^{-1}; BGB: Mg ha^{-1}.*

Connecting text to Chapter 6

Based on the modelling results from Chapter 4 and Chapter 5, it was concluded that RZWQM2 was capable of predicting the GHG emissions in eastern Canada region under water table management and different sources of N fertilizer. In Chapter 6, future climate data generated from eleven GCM-RCM models were implemented into the calibrated and validated RZWQM2 in both two sites to investigate climate change impact on GHG emissions, crop production and water quality. The effects of integrated and each single weather variables on the interactions of water, soil, nutrients and crops were quantified on field scale in Eastern Canada. The following manuscript, co-authored by Dr. Zhiming Qi, Lulin Xue, and Melissa Bukovsky, is under preparation and will soon be submitted. All literature cited in this chapter is listed in the reference at the end of this thesis.

Jiang, Q., Qi, Z., Xue, L. and Bukovsky, M., 2018. Assessing climate change impacts on greenhouse gas emissions and crop production in tile drained field using RZWQM2. To be submitted.

Chapter 6

Assessing climate change impacts on crop production, water quality, and greenhouse gas emissions in tile drained fields

Qianjing Jiang, Zhiming Qi, Lulin Xue, Melissa Bukovsky

Abstract

Increased temperature, redistributed precipitation and elevated CO_2, as results of climate change in the future, may exert essential impacts on greenhouse gas (GHG) emissions, crop water use and crop production in agricultural fields. The RZWQM2 (Root Zone Water Quality Model), driven by weather, soil, and crop information, is a process-based biophysical model which has been proven to be a promising tool to assess climate change impacts on water quality and crop production in tile drained cropland. However, it is not well documented how GHG emissions would be affected by climate change in tile drained fields. In this study, climate change impacts on crop production, water quality and GHG emissions in subsurface drained fields in two regions of Eastern Canada were assessed using calibrated and validated RZWQM2. Eleven sets of climate models were run to obtain historical (1971-1999) and future (2038-2070) daily weather data including air temperature, precipitation, solar radiation, wind speed, and relative humidity. The projected future climate data suggested that, when averaged over the output from 11 climate models, future precipitation would be increased by 8% to 9%, minimum and maximum temperature would increase by 2.4 to 2.8°C, while the changes in radiation, wind speed, and relative humidity would be minor at those two sites. Our simulated results suggested that, under future scenarios, the average drainage flow would increase by 23% - 41% (5.7- 9.1 cm), and the N losses through subsurface drains, in the meantime, would be increased by 47% to 76% (12.8-21.7 kg N ha^{-1}). Soybean yield would be enhanced by 19% to 31% due to increased photosynthesis rates under elevated CO_2, while corn yield would be reduced by 7% because of a

shorter life cycle from seedling to maturity caused by higher temperature and faster growth rate. The N_2O emissions would be enhanced by 21% to 25% due to more denitrification and mineralization, while CO_2 emissions would increase by 16% because of more crop biomass accumulation, higher crop residue decomposition, and more microbial activity. Model results suggested that corn yield would be reduced while soybean yield increased in the future, and climate change would exacerbate environmental pollution by increasing the GHG emissions from cropland and N losses in drainage water.

Key words: agricultural models; carbon and nitrogen cycling; denitrification; mineralization, water quality; climate change

6.1 Introduction

Climate change as a controversial issue has attracted much attention from researchers in different sectors, including agriculture, economics, ecology, food security, and human health. Greenhouse gases (GHGs) released from human activities are universally recognized as the most significant driver of observed climate change since the mid-20th century (IPCC, 2013).

Canada has experienced significant climate change within the past decades. The temperature has been increased by 0.5 to 1.5 degrees during the last century in Southern Canada (Zhang et al., 2000), and it is expected to continue increasing in the future. In Quebec the temperature will increase by 3.8 ℃ in the southern part and 6.5 ℃ in the northern part by 2050 (DesJarlais et al, 2010). An increase of iceberg melting, water vapor and precipitation are usually predicted to come along with global warming, which is another result of climate change. Researchers found a worldwide decline of solar radiation ranging from 0.8% to 10.6% in different countries according to long-term records from 1950 to 1980 (Wild, 2009). Based on an analysis of historical climate data across the agricultural region of the Canadian Prairies between

1951 and 2005 from 7 locations, it showed a decreasing trend of solar radiation, increasing trend of daily temperature, annual precipitation and number of rainfall events (Cutforth and Judiesch, 2007).

While climate is affected by GHG emissions, the changed climate is also predicted to result in more GHG emissions from agricultural soils because the biochemical processes that produce N_2O, CO_2 and CH_4 are affected by soil temperature and soil water. Many experiments have indicated that soil moisture and soil temperature are key factors that affect the GHG emissions (Cárdenas et al., 1993, Schindlbacher et al., 2004, Schaufler et al., 2010, Luo et al., 2013). Therefore, the future climate will have strongly influence GHG emissions due to warming temperature and changing precipitation pattern. Modelling results have indicated corn grain yield losses under climate change if no adaptation method is taken (Tao et al., 2009; Bassu et al., 2014; Wang et al., 2015). Increasing temperature is reported to negatively affect maize and wheat yields due to faster crop growth rates, shortened crop life cycle duration, earlier maturity, less CO_2 assimilation and reduced biomass production (Rosenzweig, 1990; Bassu et al., 2014). Increasing precipitation resulted in higher photosynthetic rates and crop yields in the Great Lake region of the Midwestern U.S (Southworth et al., 2000). Meanwhile, the increasing atmospheric CO_2 concentration enhances plant growth. Based on over 430 observations of crop yield for 37 species during 64 years, the enriched CO_2 concentration resulted in a 28% increase in crop yield, and a doubling of CO_2 concentration increased mean yields of C_3 crops by 33% (Kimball, 1983).

Agricultural system models provide the possibility of assessing future climate change impacts on greenhouse gas emissions, water quality and crop production in agricultural fields. Numerous agricultural models have been developed to investigate climate change impacts on hydrologic cycles, GHG emissions and crop productivity, such as DNDC (Smith et al., 2013; He et al., 2018), SWAT (Teshager et al., 2016), DAYCENT (Rafique et al., 2014) and RZWQM2 (Wang et al., 2015). Such modeling studies have indicated that soil CO_2 release and soil carbon mineralization would be significantly affected by temperature and precipitation in the future (Raich and Potter, 1995, Wang et al., 2010; Rafique et al., 2014). Mera et al. (2006) reported that yield and evapotranspiration were most sensitive to precipitation while radiation showed a nonlinear response and was not as prominent. Smith et al. (2013) assessed the climate change impact on GHG emissions and crop production in Canada using the DNDC model and demonstrated that future climate would be more favorable for crops in Canada with increasing temperature and elevated atmospheric CO_2 concentration. He et al. (2018) also applied the DNDC model to investigate the climate change impacts on crop yields and N_2O emissions in Southwestern Ontario and indicated the maize yields would be increased due to the benefits from higher temperatures for maize under climate change and elevated atmospheric CO_2 concentration significantly increased soybean yields. However, Wang et al. (2015) used RZWQM2 and stated that soybean yield would be increased by 28% because of CO_2 enrichment. Corn yield decreased by 14% due to higher temperature and shorter life cycle if the same cultivar were to be planted in 2055 in Iowa. To mitigate the negative effects of higher temperature on crop yield, He et al. (2018) suggested using new cultivars with higher thermal degree days which could increase the winter wheat yield by 39.5% with increasing biomass accumulation and higher crop N uptake in the future, and meanwhile significantly reduce N_2O emissions as well. Wang et al. (2015) found that it would be challenging for Iowa to address the water quality issue in the future since the N losses in drainage would be increased by 33.4% because of increasing drainage from higher precipitation, more N loss through higher nitrification and mineralization due to rising temperatures.

RZWQM2 is a comprehensive one-dimensional model which can be used to study the interaction of physical, chemical, and biological processes within the soil profile, including the movement of water, nutrients, and pesticides, as well as crop growth in the field under various management practices (Ahuja et al., 2000). It has been modified by Fang et al. (2015) to simulate N_2O emissions from nitrification and denitrification, and tested by Gillette et al. (2017) in predicting the tillage effects on N_2O emissions in an irrigated corn field in Colorado. The modified RZWQM2 has also been applied by Wang et al. (2016) to test different management practices in mitigating the negative effects of climate change on N losses in drainage and crop production. When simulating the N_2O and CO_2 emissions in Southern Quebec by Jiang et al. (2017), judged it to be satisfactory in predicting the GHG emissions, soil water content and soil temperature. Jiang et al. (unpublished) compared the performance of RZWQM2 and DNDC model in simulating N_2O and CO_2 emissions, crop yield and drainage, indicating that RZWQM2 has better ability in predicting the water balance and CO_2 emissions from a subsurface drained field in Harrow, Ontario and comparable performances in simulating N_2O emissions and crop productions as DNDC.

In this paper, our objective was to use the calibrated and validated RZWQM2 to assess the climate change impacts on future GHG emissions, water cycle and crop production in two subsurface-drained fields in Eastern Canada. We highlighted the quantification of annual N_2O and CO_2 emissions under projected future climates on the field scale in Eastern Canada, and the effects of each single weather variable on water cycles, water quality and crop production.

6.2. Materials and methods

6.2.1 Climate information

Daily weather data required for running RZWQM2 included precipitation, minimum and maximum temperature, wind speed, solar radiation and relative humidity. The historical weather data were obtained at Coteau-du-Lac (Station ID: 7011947) and Harrow (Station ID: 6133360) from Environment Canada. In this study, eleven coupled General Circulation Models and Regional Climate Models (GCM-RCM) were used to generate different climatic scenarios (Table 1 and 2) for 2038 to 2070. These future climate data were generated by The North American Regional Climate Change Assessment Program (NARCCAP), an international program that uses regional climate models (RCM), coupled global climate model, and time-slice experiments to generate climate scenarios and meet the research needs in United States, Canada, and Northern Mexico (Mearns et al., 2007). Since RZWQM2 failed to simulate the corn growth using the projected future climate data due to predicted frost days in growing seasons, historical climate data from 1971 to 1999 was also generated to obtain the monthly difference between future and historical weather variables. Then average changes of each month's daily temperature (℃), percent change (%) of precipitation, solar radiation, relative humidity, and wind speed were applied to the scenarios using observed historical weather from 1971 to 2000 and 1981 to 2000 in St Emmanuel (SE) site and Harrow (HR) site, respectively. The atmospheric CO_2 concentration was set at 548 ppm for the future scenarios (2038 to 2070), 344 ppm for historical scenarios of St Emmanuel (1971 to 2000, centered in 1985) and 353 ppm for Harrow (1981 to 2000, centered in 1990). Detailed methods for generating future scenarios can be found in the Supplementary Material from Wang et al. (2015).

6.2.2 Site Description

6.2.2.1 St. Emmanuel site

This 4.2 ha field is located at Coteau-du-Lac in Southern Quebec, Canada (latitude 45.32^o, longitude -74.17^o). The soil at this site is Soulanges very fine sandy loam with 5.0% organic matter in the top layer (0-0.25 m), followed by layers of sand clay loam with 1.5% organic matter (0.25-0.55 m) and clay layers with little organic matter content (0.55-1.0 m). The subsurface drained plots (75 m $\times$ 15 m) were grouped in three blocks, each housing two water table management regimes. The subsurface drains for conventional drainage were installed at a depth of 1.0 m on a 0.5% slope. N fertilization was applied each year before the seeding date for corn. Planting densities were 89,000 and 450,000 seeds ha^{-1} for corn and soybean, respectively. Detailed agronomic management for the experiment was described in Jiang et al. (2017)

6.2.2.2 Harrow site

The subsurface drained and corn-soybean rotated field was located in Southwestern Ontario (42°13′ N, 82°44′ W). The soil type was Brookston clay loam with average soil bulk density around 1.34 g cm^{-3} and porosity 52.4%. The fractions of clay, sand and silt in the soil were 37%, 28% and 35%, respectively. The saturated hydraulic conductivity was ranging from 0.07 to 0.50 cm per hour (Lu, 2015). The field slope was 0.5% on average. The tile drains were installed at the soil depth of 0.85 m, and tile drainage volume was collected in an instrumentation building using tipping buckets. Each tipping bucket was connected to a data logger and the signals of tipping rates were converted into drainage volumes.

6.2.3 RZWQM simulations

RZWQM2 was calibrated and validated using the observed soil water content, soil temperature, and N_2O and CO_2 emissions from 2012 to 2015 at St. Emmanuel (SE), Quebec

(Jiang et al, 2017), while in Harrow (HR), Ontario the daily drainage and crop yield were also included (see in Chapter 4). The statistical analysis suggested a satisfactory performance of RZWQM2 in simulating the GHG emissions at the SE site, while the predicted daily drainage, crop yield and accumulated GHG emissions were also within the acceptable range at the HR site. Subsurface drains were set at 1 m and 0.85m depth in SE and HR sites, and N fertilizer was applied each year at 200 kg ha^{-1} before the planting date for both sites. Corn and soybean were rotated by running each scenario twice, corn in odd years in one run and soybean in odd years in the other, to ensure both corn and soybean were planted in every simulated year. Planting and harvesting dates were adjusted based on the field experiment. The corn and soybean were planted on May 1st and harvested on October 15th each year at the SE site, while at the HR site, both corn and soybean were planted on May 25th and harvested on November 15th and October 15th for corn and soybean, respectively. RZWMQ2 was run under the baseline scenario firstly, and then the 11 sets of differences in temperature, precipitation, wind speed, solar radiation, and relative humidity were added to the baseline to generate future climate scenarios. The 11 full sets of climate data were run first with all factors in combination, then runs were done in which only one weather variable was changed at a time to investigate the single impact of these factors on hydrology, GHG emissions and crop production. Model output included the hydrology components, nutrient components and crop growth conditions, which were evapotranspiration, drainage rate, runoff, lateral flow, crop yield, crop maturity days, GHG emissions and N losses.

6.3. Results and discussion

6.3.1. Climate scenarios

The annual average baseline and projected future climate variables for St. Emmanuel and Harrow are listed in Table 6.1. Generally, future annual precipitation would increase by 8%, and minimum temperature and maximum temperature would rise by 2.9 ℃ and 2.4 ℃ for St. Emmanuel. Wind speed would increase by 1.5%, while solar radiation and relative humidity would decrease slightly by 2.4% and 0.4%, respectively. Similar predictions have been reported by DesJarlais et al (2010) for Southern Quebec, indicating that temperature would increased by 2.5 ℃ to 3.8 ℃ in winter and 1.9 ℃ to 3.0 ℃ in the summer, while precipitation is expected to increase by 8.6% to 18.1% in winter with no change in summer. Similarly, the minimum and maximum temperature is expected to increase by 2.8 ℃ and 2.5 ℃, respectively in Harrow site. The precipitation in Harrow would increased by 9%, while changes of wind speed, solar radiation and relative humidity would be very minor. The historical average annual precipitation was 88 cm, while the projected average future precipitation would be 96 cm (+8 cm) from 2038 to 2070. Our projected future temperature and precipitation in Harrow was comparable to previous studies at nearby Woodslee, ON, which is 34 km away from Harrow. For example, Smith et al. (2013) indicated that future annual temperatures would increase by 3.5 ℃ and precipitation would increase by 5 cm for 2041 to 2070. He et al. (2018) stated that future precipitation would increase by 2 cm and 9.7 cm while temperature would increase by 3.5 and 5.7 ℃ as predicted by RCP 4.5 and RCP 8.5 models.

6.3.2. Integrated future climate impact on crop production, water quality and GHG emissions

Taking into consideration all the changes in climate variables, our simulation showed that the production of corn will decrease by 7% while soybean will benefit significantly from climate change by 31% in the future in Southern Quebec, and in Southwestern Ontario the corn yield will decrease by 7% while soybean yield will increase by 19% (Table 6.2). The reduction in corn yield will result from higher temperature and shorter growing days from grain filling to maturity. The evapotranspiration will increase slightly, since increasing evaporation caused by increasing temperature will be balanced by decreased transpiration because of the closure of stomata in response to elevated CO_2. Drainage will increase by 23% in SE and 41% in HR (figure 6c), with the majority of the increased drainage in the months of January, February and December, as a result of increasing precipitation and warming winter seasons.

Our simulated annual N losses in subsurface drainage from SE and HR were 46 and 20 kg N ha^{-1}, which were comparable to previous studies in or near the experimental sites. The measured NO_3-N losses in a field in the Pike River watershed, Quebec was 31.9 kg N ha^{-1} in 2002-2003 and 40.7 kg N ha^{-1} in year 2003-2004 (Gollamudi et al., 2007), and Madramootoo et al. (1992) observed the total N losses at 36 and 70 kg N ha^{-1} during the growing seasons (from April to November) in two subsurface drained potato fields at St. Leonard d'Aston, Quebec in 1989 and 1990. Patni et al. (1996) reported 13 to 30 kg N ha^{-1} losses of N in tile drains from corn fields in Southwestern Ontario. With changes in all the weather variables considered, the study areas would face a sever challenge in water quality in the future due to 47% and 59% more N losses in drainage for the SE and HR sites, respectively. Higher temperatures and elevated atmospheric CO_2 concentrations in the future enhance microbial activities or promote crop growth, leading to more denitrification (+31.5% in SE and +53% in HR) and mineralization (+17.7% in SE and 15% in HR) in the soil. Consequently, the increasing trend of N losses will result from the increasing precipitation, and warming temperature, but elevated atmospheric CO_2 concentration will reduce N losses in drainage due to increasing N uptake by crops. The N_2O and CO_2 emission would rise by 20.8% and 15.7% in SE, and increase by 25% and 16% in HR if no adapting management practices were taken. Our prediction of increased GHG emissions under climate change were in agreement with previous studies in North America as reported by He et al. (2018).

6.3.3. Temperature impact on crop production, water quality and GHG emissions

Monthly changes in temperature for the two sites are plotted in Figure 6.1. Both sites would experience greater minimum temperature increase in winter seasons of November, December, January and February than the other months. In HR site, the maximum temperature during the growing season only increased by 1.5 to 1.9^oC, and minimum temperature increased by 1.0 to 1.6^oC, which were lower than the monthly average increment (2.5^oC for maximum and 2.9^oC for minimum). This is supported by the observation of historical air temperature in HR reported by Tan and Reynolds (2003), who indicated that the temperature in the growing seasons from 1980 to 2000 in Southwestern Ontario showed no obvious warming trend, which was also reported in other regions in Ontario (Smith et al., 1998).

The average corn and soybean yields for over 30 years under simulated future temperature indicated that rising temperature will significantly reduce the corn yield by 27% and 18%, while soybean yield will decrease by 4% and 7% in the SE and HR sites. The negative effect of increasing temperature on crop production can be explained by shorter crop growth cycles resulted from faster grain filling and earlier maturity. Warmer temperature leads to faster development for crops, and the time for grain to mature will be reduced as a consequence (He et al, 2018). Our simulated crop life cycles (from seedling to physiological maturity) were reduced from 149 days to 122 days for corn (Table 6.3), and from 121 days to 109 days for soybean at the SE site, while at the HR site they were reduced from 146 days to 122 days for corn and from 120 days to 111 days for soybean with higher temperature in growing seasons. The reduced crop yields under increasing temperature can be mitigated using new cultivars. Smith et al. (2013) indicated higher corn yields when planting a cultivar with longer growing degree days (GDD) under a future climate scenario at the Harrow site.

Our predicted corn yield experienced more reduction than soybean because the warming temperature has very different effects on corn and soybean due to their different optimal temperatures for growth. According to several field experiments and model simulations, higher (44.8% - 93.6%) corn yield was observed and simulated from cool areas with growing season temperatures around 18.0 to 19.8^oC at Grand Junction, CO, while compared with those warmer areas such as Champaign, IL, (21.5~24 ^oC) and warm tropical sites (26.3~28.9 ^oC) in Katherine, Australia (Muchow et al., 1990). In contract to corn, soybean prefers higher growing season temperature. Its optimal temperature for post-anthesis, single seed growth rate, and for seed size are 23 ℃, 23.5 ℃, and 23 ℃, respectively. For example, in the Southern USA, where the current average growing season temperature is around 26.7^oC, the soybean yield is expected to decrease by 2.4% with a 0.8^oC temperature rise, while in the Midwest where current growing season temperature is around 22.5 ^oC, the yield may increase (Hatfield et al., 2011). A field study conducted in northern parts of Japan, which are cold regions with mean growing season temperatures ranging from 19.4 to 22.6 ^oC, reported that late maturing soybeans would benefit from a temperature increase (Kumagai and Sameshima, 2014).

The increased air temperature resulted in warmer soil temperature, which was one of the key factors modulating microbial activities. When the soil temperature rises, the decomposition of SOM will accelerate, leading to high CO_2 emissions through microbial respiration. The simulated CO_2 emission was increased by 1.9% (+77 kg ha^{-1}) and 2.0% (+121 kg ha^{-1}) in SE and HR due to the higher respiration from microorganisms and more C mineralization, while the annual total N_2O emissions increased by 9% (0.21 kg N ha^{-1}) and 14% (0.07 kg N ha^{-1}) on average for the two sites because of enhanced nitrification and denitrification. The consumption of O_2 by microorganisms from respiration resulted in ideal anaerobic conditions for denitrification, therefore, higher N_2O

emissions are tied to increasing CO_2 emissions under warmer soil conditions (Elder and Lal, 2008). Our simulated CO_2 and N_2O emissions both responded positively with increasing future temperature, which is supported by the field studied reported by Schaufler et al. (2010). The effect of warming temperature on N_2O might be greater than on CO_2, due to the coupling of microbial C and N cycle (Butterbach-Bahl et al., 2013). It should also be noted that the increasing temperature resulted in less crop residue accumulation, thus less crop residue decompostion was simulated but more soil humus decomposition still led to 2% higher CO_2 emssions.

The simulated annual actual evapotranspiration was 54.9 cm for corn and 44.4 cm for soybean under baseline, while 58.4 cm and 50.7 cm in the future scenarios at the SE site (Table 6.3). The similar trend was also simulated at the HR site, with the AET increased from 47 cm to 50 cm for corn and increased from 46 cm to 48 cm for soybean. The predicted historical ET in SE site is comparable with annual ET in the St. Esprit agricultural watershed from 53.1 cm to 56.6 cm simulated by Peters et al. (1971). And the simulated annual ET for HR site was comparable to the measured values in the years of 1992 to 1994 around 42 to 45 cm under free drainage for corn field at the same experimental site by Tan et al. (2002). The increase of evapotranspiration led to decreases of both drainage rate and runoff. Future drainage was decreased by 8% (-3.0 cm) and runoff was 18% lower (-1.6 cm) in SE site, while in HR site the drainage and runoff decreased by 2.7% (-0.6 cm) and 24% (-2.7 cm), respectively.

Although higher temperature promoted water loss from evapotranspiration and reduced the drainage water, the N losses in tile drainage will increase dramatically by 41% (+19 kg N ha^{-1}) at the SE site and 48% (+9 kg N ha^{-1}) at the HR site, because 12.2% and 10% more soil organic N (+20.1 kg N ha^{-1} and +15.3 N ha^{-1}) will be mineralized due to warming temperature in SE and

HR site, respectively (figure 2). Meanwhile, the annual denitrification rates will increase by 1.2 and 1.7 kg N ha^{-1} accordingly.

6.3.4. Precipitation impact on crop production, GHG emissions and water quality

Though simulated future annual precipitation at the SE site will increase by 8.2% on average, the distribution of precipitation changes will not be even across each month of the year (Figure 6.2). Generally, the monthly rainfall in growing season will be less affected, while in winter there will be more precipitation increment. In the months of July, August, September and October the rainfall will only increase by 3.2%, 8.2%, 2.6% and 0.4%, respectively. The simulated increase of precipitation did not show obvious impact on crop production in the field because of very minor changes of precipitation in growing season and neglectable water stress during crop's growing season in the St. Lawrence lowlands which is a semi-humid area. Therefore, the simulated future corn and soybean yields in SE will only increase by 1.1% (from 13001 kg ha^{-1} to 13140 kg ha^{-1}) and 0.2% (from 3764 kg ha^{-1} to 3771 kg ha^{-1}), respectively, assuming only change in precipitation occurs.

At the HR site, the historical annual precipitation was 88 cm and it will increase to 96 cm (9%) in the future on average. However, the distribution of the precipitation increment will also be uneven in different seasons. Tan and Reynolds (2003) had concerned about the increasing water deficit in the growing season and less crop yield in the future for this region, and our predicted results indicated that future precipitation will be 5% and 1% less in June and July while 13% and 6% more in in August and September in this region from 2038 to 2070. The changing precipitation pattern resulted in very minor effects on crop production, with corn and soybean yields increased only by 0.05% and 2%, since neglectable changes in actual and potential evapotranspiration were predicted in the future.

The predicted changes in precipitation mainly affected the hydraulic components of drainage, runoff and lateral flow. Changes in both crop transpiration and soil evaporation will be very minor with the increase of precipitation because the water stress in both regions was not the major concern. Future precipitation in SE site will increase from 97.6 cm to 105.4 cm (+7.8 cm), and the increment of drainage and runoff will be 5.4 cm (16%) and 1.8 cm (19%), respectively, which means 92% of the extra precipitation will go to the drainage and runoff. Similarly, the precipitation will increase by 8 cm (9%) in HR site, meanwhile the drainage and runoff will increase by 5.5 cm (26%) and 2.2 cm (6%), respectively as a consequence. While the ET for both corn and soybean will not be significantly affected by the increasing precipitation, relationship between increased precipitation, increased annual tile drainage rate and runoff from 11 models, can be expressed with the linear equations as shown in Figure 6.3. Similar simulated results for linear relationship between increased precipitation and drainage have been reported by Wang et al. (2015). The increasing precipitation and thereby higher drainage resulted in more N losses in drainage, which increased by 9.3% (from 46.6 to 51.0 kg N ha^{-1}) at SE and 13.8% at HR (from 21.6 to 24.5 kg N ha^{-1}) sites, indicating the potential negative impact of future precipitation on water quality issues.

Despite the fact that rainfall events play an important role in affecting the microbial activities and thereby stimulate GHG emission, the simulated future mineralization, denitrification, CO_2 and N_2O emission all changed within only 1%. Although the GHG emissions were expected to be very sensitive to precipitation events, the long-term changes in precipitation did not significantly affect GHG emission on global scale (Del Grosso and Parton, 2012). In this simulation, our daily average increment of precipitation was around 0.3 and 0.2 mm at the SE and HR sites, and the majority of the extra water (92% for SE and 98% for HR) will go to the tile drainage, lateral flow and runoff, which means the changes of soil water storage will be very minor. Therefore, the simulated future precipitation pattern and amount will not have great effects on GHG emissions.

6.3.5. Elevated CO_2 impact on crop production, GHG emissions and water quality

Our simulation indicated that both corn and soybean yield will benefit from the enriched atmospheric CO_2 concentration in the two sites. The predicted yields for corn were 13001 kg ha^{-1} and 10360 kg ha^{-1} for SE and HR sites under baseline (Table 6.4), while in the future the yield will increase by 14.4% (14880 kg ha^{-1}) and 15.0% (11910 kg ha^{-1}), respectively. The soybean yields will increase by 29.9% and 30.3% for SE and HR sites, which were more affected by the elevated atmospheric CO_2 concentration than the corn. Our predicted results were comparable to the simulation by He et al. (2018), who predicted 9.3% to 17.1% higher corn yields and 17.4% to 33.5% higher soybean yields under elevated atmospheric CO_2 concentration in the future (2071-2100) than historical (1971- 2000) yields for Woodslee, ON. Hatfield et al. (2011) also indicated that doubling the CO_2 atmospheric concentration would result in 30% increase of C3 crop yields (soybean is a C3 crop), and less than 10% increase of C4 crop yields (corn is a C4 crop). Our prediction is supported by a research conducted by Kimball (1983), who reported mean increase of soybean yield by 27% based on 12 observations when doubling the atmospheric CO_2 concentration. However, the weed growth would also be promoted, which could trade off the yield increment from elevated CO_2 concentration (Ziska, 2000), and the application of more herbicide could result in water quality problem.

The impact of elevated atmospheric CO_2 concentration on water cycle mainly reflects on the crop's water use. The basis for rising CO_2 concentration as fertilization is through affecting crop's photosynthesis and stomatal conductance, therefore to increase the yield and decrease water uptake (Long et al., 2006). Changes on crop's growth, LAI, leaf stomatal aperture and conductance for water loss, and water vapor pressure gradient are all factors that affect crop's transpiration. In DSSAT-CERES model, the stomatal conductance decreases when increasing CO_2 concentration therefore reduces the plant transpiration (Ko et al., 2012). In our study, the elevated atmospheric CO_2 concentration led to reduction of the actual transpiration by 8% for corn to 11% for soybean at both sites. Hatfield et al. (2011) reported that the amount of measured crop's water use decreased by 2 to 13% when elevating the concentration of CO_2 depending on the species because of the closure of some leaf stomata and less water vapor loss from leaves to atmosphere. Our simulated future actual ET for corn and soybean reduced by 7.3% (-4.0 cm) and 9.1% (-4.0 cm) in SE site, and reduced by 10% (-4.7 cm) and 8% (-3.5 cm) in HR site, thus annual drainage flow and runoff increased by 10.2% (+3.6 cm) and 2.8% (+0.25 cm) in SE, and increased by 12.6% (+2.8 cm) and 2.0% (+0.1 cm) in HR site as a result of the decline of crop ET.

Our simulation suggested an increasing trend of N_2O emissions with elevated atmospheric CO_2 concentration in both two sites, which were 13% and 17% higher than baseline in St. Emmanuel and Harrow site, respectively. Higher N_2O emission under elevated atmospheric CO_2 concentration has been reported by Baggs et al. (2003), Kettunen et al. (2005), Bhattacharyya et al. (2013) and Wang et al. (2018). This could be explained by more easily decomposable root exudates resulted in enhanced microbial activities in soil (Kettunen et al. 2005), thereby increasing nitrification and denitrification. In addition, increased C allocation from root biomass and exudation provided the energy for denitrification (Baggs et al., 2003). In the present study, the simulated denitrification increased by 21% and 24%, the annual N_2O emission from denitrification increased by 14% and 22%, and the N_2O emission from nitrification also increased by 12% and 14% at the SE and HR sites, respectively. Although the enhancement of N_2O emission was usually expected with elevated CO_2 emission (Holmes et al., 2006; Bhattacharyya et al., 2013; Wang et al., 2018), some modeling results and FACE (free air carbon dioxide enrichment) experiments supported an argument that higher crop N demand might reduce the soil N and microbial availabilities, leading to lower denitrification and nitrification thus decreasing N_2O emission (Hungate et al., 1997, Reich et al., 2006, Xu-Ri et al., 2012; He et al., 2018).

Simulated average annual N mineralization will increase by 14.3 kg N ha^{-1} from 170.0 kg N ha^{-1} to 184.3 kg N ha^{-1} in SE site, and in HR site it will increase from 155 to 175 kg N ha^{-1}. The increased C and N mineralization was resulted from higher accumulated crop residue from each year, leading to 15% and 18% higher CO_2 emission in SE and HR sites from soil. Our results were supported by Rafique et al (2014), which indicated that the predicted changes in crop yield could be the reason for increasing/decreasing of GHG emissions due to the changes of soil C dynamics. De Graaff et al. (2006) also demonstrated the increase of CO_2 respiration from soil due to the stimulation of increased total plant biomass by elevated atmospheric CO_2 concentration. Although the elevated atmospheric CO_2 concentration resulted in higher mineralization and more denitrification, as well as increasing drainage flow, the N losses in drainage were reduced by 6% and 16% in two sites. This might be due to the increasing N assimilation of crops. The simulated N uptake by corn will be increased by 5% (from 288 to 304 kg N ha^{-1}) and 13% (from 283 to 321 kg N ha^{-1}) for SE and HR sites, respectively, and soybean N uptake increases by 30% (from 336 to 436 kg N ha^{-1}) and 32% (from 408 to 538 kg N ha^{-1}) for the two sites. The extra N uptake of soybean was mainly resulted from the enhanced N fixation by soybean (from 200 to 294 kg N ha^{-1} in SE site and from 270 to 392 kg N ha^{-1} in HR site).

6.3.6 Solar radiation, relative humidity and weed speed impact on crop production, water quality and GHG emissions

The simulated future solar radiation has limited impact on corn and soybean yields. The average daily radiations of baseline were around 13 MJ m^{-2} in both two sites, while in the future they were expected to decrease by 2% and 5% in SE and HR sites. The reduced radiation resulted different responses to crop production in the two sites, which suggested 3% yields reduction in HR, while in SE site crop yields increased by 2%. This could be explained by different seasonal patterns of radiation changes in the two regions. The future average daily radiation during crop growing period (from planting date to physical maturity date) rose by 3% to 7% in SE site, while in HR site the radiation reduced by 3% to 8%. Consequently, as affected by the declined radiation, the simulated corn and soybean yields in HR site were reduced by 3% in the future, however, future yields for corn and soybean were 1.4% and 2.0% higher than baseline Increased crop yields in SE resulted in slightly more crop residue decomposition and GHG emissions while in HR site the results were the opposite. However, changes in CO_2 and N_2O emission for both sites were within 2% due to the minor changes in yields.

The future predicted wind speeds will be 1.5% lower and 0.4% higher than baselines at the SE and HR sites, respectively. Very limited differences for crop production (within 1% in SE and 0.1% in HR sites) were found under changing wind speed. Reduced wind speed resulted in lower soil evaporation (within 0.5%) in SE site, while in HR site the soil evaporation changed within 0.01%. The GHG emissions will be limitedly affected by the wind speed (within 0.3% and 0.1% for SE and HR sites).

The predicted relative humidity was 2.4% lower and 1.5% higher in SE and HR sites. No changes were found for simulated GHG emissions, water balance or crop yields with minor changes in relative humidity under the future climate scenarios.

6.4. Summary and conclusion

Our simulated results suggest that higher future precipitation mainly affected the drainage and runoff but not crop yield because almost no water stress was simulated for crops in the two regions. The increased temperature will lead to higher evapotranspiration; therefore, less water will be drained out from the field and less runoff was estimated as well. However, higher temperature will enhance mineralization and denitrification in soil profile, leading to more N losses in drainage water and more GHG emissions from soil. Meanwhile, higher temperature will accelerate the crop growth rate and shorten the growth lengths for both corn and soybean, which results in lower crop yields for both corn and soybean. Furthermore, higher temperature will have more significant effects on reducing corn yield (17%-27%) than soybean (4%-7%) due to different optimal growing temperatures for the two crops. Elevated atmospheric CO_2 will result in the closure of some leaf stomata, thus decrease the plant water uptake and water vapor from the leaves to the air. For the crop production, it affects corn (C4 crop) and soybean (C3 crop) in different ways. The predicted yields for corn and soybean in both Ontario and Quebec would rise by around 15% and 30%, respectively. Soybean yield will be increased dramatically because increasing atmospheric CO_2 concentration will lead to direct increase of net photosynthetic CO_2 uptake, while minor increase of corn yield was predicted as increasing CO_2 only increases water use efficiency through decreasing the stomatal conductance. The hydraulic cycle, GHG emissions from soil and crop production were found to be not very sensitive to the future solar radiation, relative humidity and wind speed because the changes of those climate variables will be minor.

In conclusion, three future climate variables will be strongly associated with corn and soybean production: temperature, precipitation and atmospheric CO_2 concentration. Increasing future temperature will result in crop yield reductions, especially for corn, but the negative impact of increasing temperature on crop production can be solved by replacing cultivars with longer life cycles (Smith et al, 2013; Wang et al., 2016). Nevertheless, future temperature will also exacerbate the problem of N losses in tile drainage and GHG emissions by affecting the soil microbial activities. Agronomic management practices should be considered for the future environmental problems. Elevated atmospheric CO_2 concentration will improve crop productivities, but also enhance GHG emissions because of more crop residue left in soil for decomposition. The future precipitation will not affect the crop productions, and the extra water will be drained out directly from soil surface or through tiles, leading to more N losses to drainage water. The future study should be focused on the mitigation and adaptation strategies for the climate change impact on GHG emissions, crop production and water quality in Eastern Canada based on current simulations.

Table 6.1. Annual average weather variables of precipitation (P), minimum temperature (T_{min}), maximum temperature (T_{max}), wind speed (U), solar radiation, and relative humidity (RH) for baseline and future scenarios at (a) St. Emmanuel, Quebec and (b) Harrow, Ontario

Site	weather	P cm	T_{min} ℃	T_{max} ℃	U km d^{-1}	Radiation MJ m^{-2} d^{-1}	RH %
a	baseline	98	1.9	10.7	342	13	71
	CRCM-ccsm	97	1.9	10.7	342	13	71
	CRCM-cgcm3	102	5.0	13.3	338	13	71
	ECP2-gfdl	106	4.7	13.2	340	13	72
	HRM3_gfdl	114	4.8	12.9	343	13	72
	HRM3_hadcm3	107	4.9	13.9	343	13	67
	MM5I_ccsm	98	4.7	13.4	342	12	69
	MM5I_hadcm3	113	4.6	12.7	329	11	71
	RCM3_cgcm3	106	5.7	13.4	311	11	71
	RCM3_gfdl	108	4.7	13.3	334	10	71
	WRFG_ccsm	104	4.2	12.8	332	10	71
	WRFG_cgcm3	95	4.9	13.2	328	11	70
	Future average	108	4.8	13.1	366	12	70
	Difference	+8%	+2.8	+2.4	-1.5%	-2%	-0.4%
b	baseline	88	5.4	13.8	336	13	78
	CRCM-ccsm	92	8.3	16.4	342	12	79
	CRCM-cgcm3	98	8.3	16.4	327	12	80
	ECP2-gfdl	88	7.9	16.1	332	12	78
	HRM3_gfdl	97	8.4	16.5	331	13	80
	HRM3_hadcm3	105	8.9	17.1	319	12	80
	MM5I_ccsm	96	8.6	16.4	316	12	79
	MM5I_hadcm3	93	9.2	16.9	330	13	79
	RCM3_cgcm3	102	8.2	16.4	321	13	80
	RCM3_gfdl	89	6.4	14.8	330	13	78
	WRFG_ccsm	105	9.3	17.1	323	12	81
	WRFG_cgcm3	95	6.9	15.0	328	12	79
	Future average	96	8.2	16.3	336	12	79
	Difference	+9%	+2.8	+2.5	-3%	-5%	+1%

Table 6.2. Simulated average annual crop yields, GHG emissions, N transformations in St. Emmanuel and Harrow sites for baseline and future scenarios under integrated future change

	St. Emmanuel		Harrow	
	baseline	$Future_{avg}$	baseline	$Future_{avg}$
N_2O emission (kg N ha^{-1})	2.3	2.8	0.9	1.1
Denitrification (kg N ha^{-1})	11.5	15.2	4.5	7.1
Mineralization (kg N ha^{-1})	169	199	155	171
N in drainage (kg N ha^{-1})	46	68	22	34
CO_2 emission (Mg ha^{-1})	4.3	5.0	4.9	5.8
ET-corn (cm)	55	56	47	43
ET-soybean (cm)	44	46	46	43
Drainage (cm)	35	41	22	21
Corn yield (Mg ha^{-1})	13.0	12.9	10.4	9.5
Soybean yield (Mg N ha^{-1})	3.8	4.9	3.6	4.3

Table 6.3. Simulated average annual crop yields, GHG emissions, crop life cycles, N transformations in St. Emmanuel and Harrow sites for baseline and future scenarios under changing temperature

	St Emmanuel		Harrow	
	baseline	$Future_{avg}$	baseline	$Future_{avg}$
N_2O emission (kg N ha^{-1})	2.3	2.8	0.9	1.0
Denitrification (kg N ha^{-1})	11.5	15.2	4.5	6.2
Mineralization (kg N ha^{-1})	169	184	155	171
N in drainage (kg N ha^{-1})	46	71	22	32
CO_2 emission (Mg ha^{-1})	4.3	4.3	4.9	5.1
ET-corn (cm)	55	58	47	49
ET-soybean (cm)	44	51	46	48
Drainage (cm)	35	32	22	21
Corn life maturity (day)	149	122	146	122
Soybean maturity (day)	121	109	120	111
Corn yield (Mg ha^{-1})	13.0	9.4	10.4	8.5
Soybean yield (Mg N ha^{-1})	3.7	3.6	3.6	3.4

Table 6.4. Simulated average annual crop yields, GHG emissions, N transformations in St. Emmanuel and Harrow sites for baseline and future scenarios with elevated CO_2 concentration

	St Emmanuel		Harrow	
	baseline	$Future_{avg}$	baseline	$Future_{avg}$
N_2O emission (kg N ha^{-1})	2.3	2.6	0.9	1.0
Denitrification (kg N ha^{-1})	11.5	14.0	4.5	5.5
Mineralization (kg N ha^{-1})	169	184	155	175
N in drainage (kg N ha^{-1})	46	44	22	18
CO_2 emission (Mg ha^{-1})	4.3	5.0	4.9	5.8
ET-corn (cm)	55	51	47	42
ET-soybean (cm)	44	40	46	42
Drainage (cm)	35	39	22	25
Corn yield (Mg ha^{-1})	13.0	14.8	10.4	12.0
Soybean yield (Mg N ha^{-1})	3.8	4.9	3.6	4.7

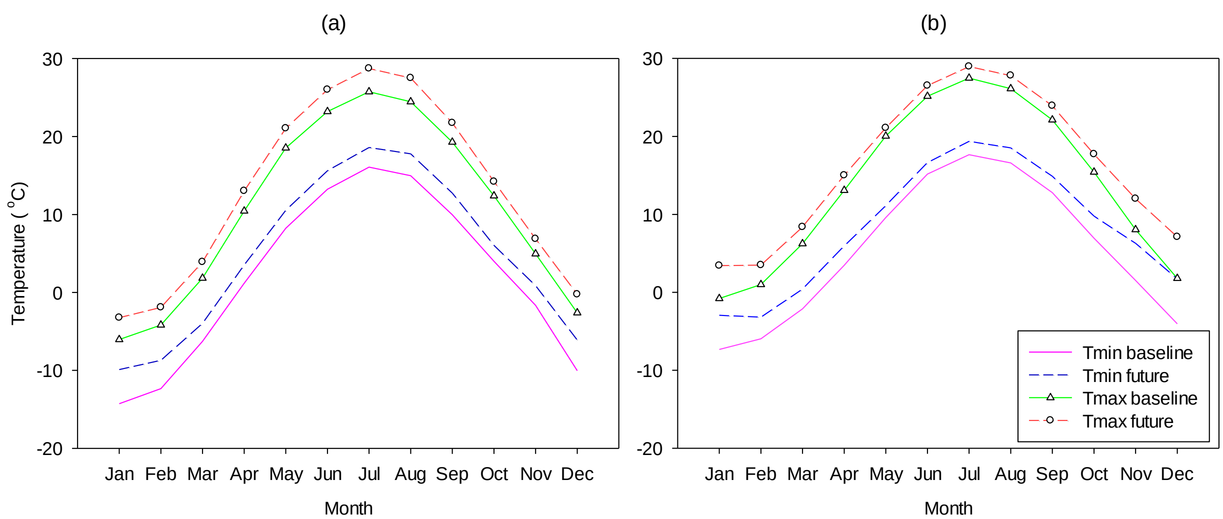

Figure 6.1. Projected average monthly minimum and maximum temperature for baseline and future scenarios at a) St. Emmanuel and b) Harrow site.

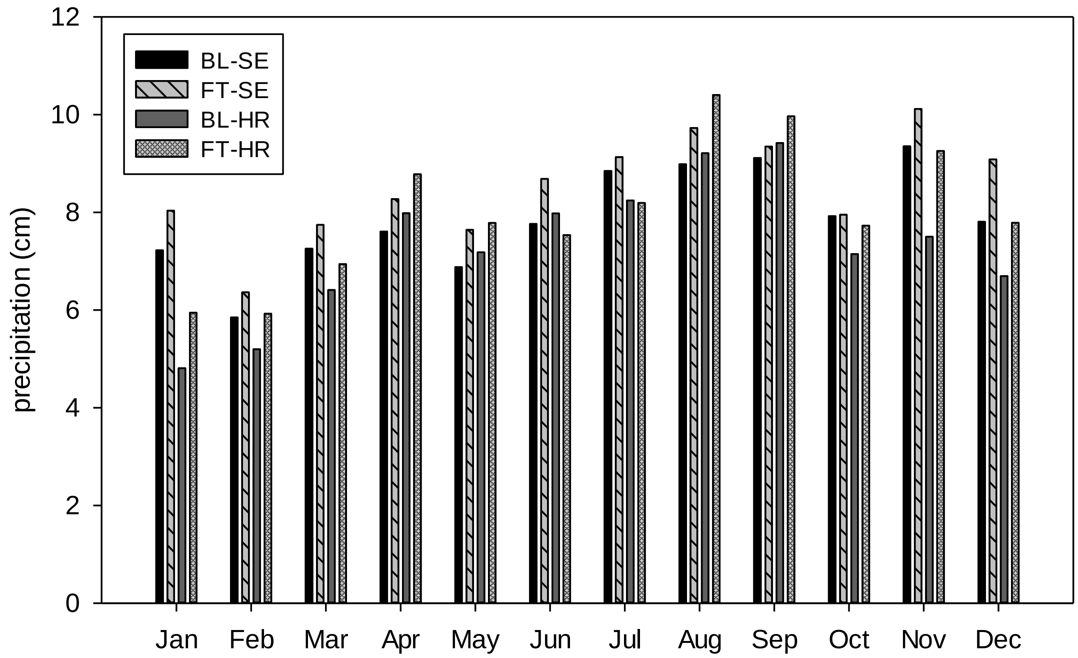

Figure 6.2. Monthly distribution of baseline (BL) and future (FT) precipitation for St. Emmanuel site (SE) and Harrow site (HR).

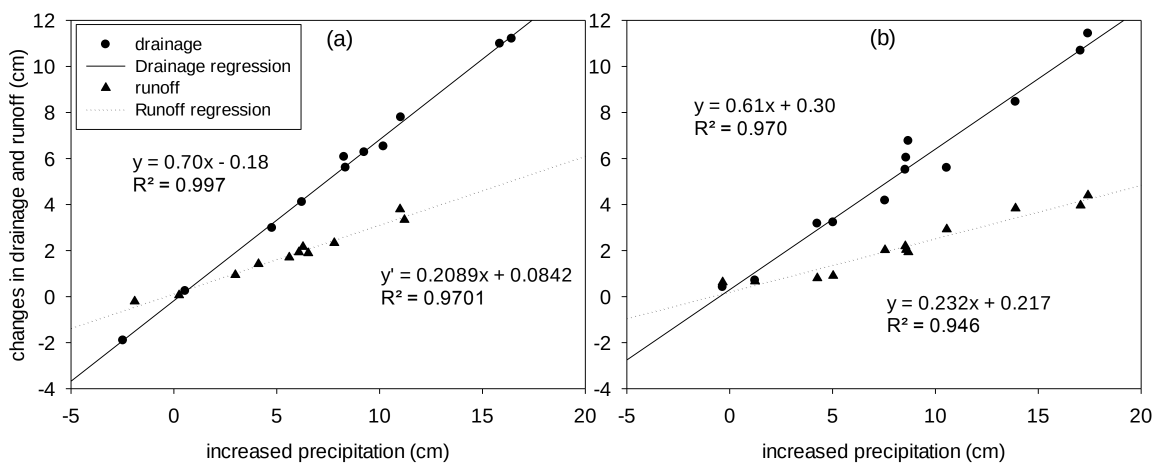

Figure 6.3. The relationships between increased precipitation, drainage and runoff in (a) St. Emmanuel and (b) Harrow sites. The dots and triangles are values from 11 scenarios.

Chapter 7

General summary and conclusions

7.1 General summary

The overall goal of the research was to quantify the interactions between agricultural management, climate change, crop growth, and environmental quality and provide mitigation strategies for greenhouse gas emissions in subsurface drained fields. The RZWQM2 modelling approach was applied in this research to assess the agronomic practices and climate change impact on crop yields, water quality, water balance, and GHG emissions. To this end, a few model evaluations, applications and future predictions under climate change in Southern Quebec and Southwestern Ontario were undertaken to address research objectives.

7.2 Conclusions

Objective 1: To evaluate the hydrologic component of RZWQM2 (Root Zone Water Quality Model) using a comprehensive hydrological dataset including subsurface tile drainage, sub-irrigation, soil water content, sap flow and crop growth data such as leaf area index, crop yield and crop growth stages

While mean values for growing season tile flow under both free drainage (FD) and controlled drainage with subirrigation (CD-SI) were reasonably accurate, winter tile flow was significantly overestimated, indicating RZWQM2's reliability to be compromised by its imperfect winter drainage process. Accordingly, a Kalman filter technique was applied to enhance model reliability and reduce predictive uncertainties. A novel RZWQM2 model equipped with a Kalman filter algorithm adequately simulated, in both calibration and validation phases, the hydrology and corn growth which occurred under both FD and CD-SI systems at the selected field site. Simulation results suggest that RZWQM2 model can be used for water management under subsurface drained and irrigated field and the Kalman filter technique significantly improved the accuracy of RZWQM2 model in simulating winter drainage in cold areas.

Objective 2: To test RZWQM2's ability to predict GHG emissions in subsurface drained field under water table management

The Root Zone Water Quality Model 2 (RZWQM2) was calibrated and validated for the estimation of N_2O and CO_2 emissions. It performed satisfactorily in predicting soil temperature, soil water content (SWC), N_2O and CO_2 emissions under free drainage and controlled drainage with sub-irrigation in southern Quebec, except for a less satisfactory simulation of N_2O emission during the validation period due to the failure to predict an extreme value after a heavy rainfall event.

Objective 3: To compare the performance of the RZWQM2 and DNDC models for in simulating GHG emissions, crop yield and drainage flow from in a subsurface drained and corn-soybean rotated field under water table and N management.

RZWQM2 is an agricultural system model which comprehensively handles crop growth, hydraulic cycles and nutrient cycling in field scale, and DNDC is specialized for nutrient cycling but also had good ability in simulating SWC, drainage and crop growth. Both models provided reliable estimation of cumulative N_2O emission under different treatments over four years, but RZWQM2 performed much better than DNDC in predicting the daily CO_2 emissions. Overall, RZWQM2 requires very experienced users for calibration and validation due to the uncertainty and complexity of parameters and is more computation intensive, while DNDC model is more user-friendly and works well with simple calibration. It is important to test the hydraulic components of agricultural system models to better understand the complicated interaction between soil, water and nutrients. Therefore, improvements are suggested for DNDC model in computing the soil water dynamics.

Objective 4: To use RZWQM2 to investigate the impacts of different agronomic management practices on long-term annual GHG emissions and propose some mitigation and adaptation suggestions based on the model simulations

The optimal range of N fertilization in the range of 125 to 175 kg N ha^{-1} was proposed to obtain higher NUE (nitrogen use efficiency, 7-14%) and lower N_2O emission (8-22%) with minor yield reduction (2-9%), compared to 200 kg N ha^{-1} for corn-soybean rotation. The long-term average annual N_2O and CO_2 emissions were estimated to be 2.16-2.55 kg N ha^{-1} and 3854-3887 kg ha^{-1} with 125- 175 kg N ha^{-1} of dry urea fertilization under free drainage and corn-soybean rotation. While remaining crop yields, splitting N application into two dates (one before planting and the other two weeks before silking) would potentially decrease total N_2O emission by 11.0 %, but CO_2 emission was only reduced by 0.3%. Due to higher soil moisture and lower soil O_2 under controlled drainage with sub-irrigation (CD-SI), CO_2 emissions declined by 6% while N_2O emissions increased by 21% compared to free drainage (FD). A corn-soybean rotation reduced CO_2 and N_2O emissions by 18.8% and 20.7%, respectively, when compared with continuous corn production. This study concludes that RZWQM2 model is capable of predicting GHG emissions, and GHG emissions from agriculture can be mitigated using agronomic management.

Objective 5: To use the calibrated and validated RZWQM2 to assess the climate change impacts on future GHG emissions, water cycle and crop production in Eastern Canada

Three future climate variables were strongly associated with corn and soybean production: temperature, precipitation and atmospheric CO_2 concentration. Increasing future temperature would result in crop yield reductions, especially for corn, but the problem of its negative impact on crop production can be easily solved by using cultivars with longer growing degree days. Nevertheless, future temperature would also exacerbate the problem of N losses in tile drainage and GHG emissions by affecting the soil microbial activities. Agronomic management practices should be considered for the future environmental problems. Elevated CO_2 concentration would improve crop productivities, but also enhance GHG emissions because of more crop residue left in soil for decomposition. The future precipitation would not affect the crop productions, and extra water would be drained out directly from soil surface or through tiles, leading to more N losses to drainage water. Model results suggested that corn yield would be reduced while soybean yield increased in the future, and the climate change would exacerbate environmental pollutions by increasing the GHG emissions from cropland and N losses in drainage water.

7.3 Contributions to knowledge

Based the objectives of this research, this thesis provides following contributions to knowledge:

1. The agricultural system model, RZWQM2, has been comprehensively tested for its hydraulic, nutrient and crop growth components. Meanwhile, the performance of RZWQM2 has been compared with another widely used agricultural system model, DNDC. RZWQM2 was found to be more applicable for subsurface-drained fields.
2. A novel RZWQM2 model equipped with a Kalman filter algorithm was first applied for simulating the hydrology in winter.

3. Optimal range of N fertilization was recommended from 125 to 175 kg N ha^{-1} to mitigate N_2O emissions and improve NUE based on the simulation. The splitting N fertilization and rotation would help to reduce the GHG emissions, while CD-SI results in more N_2O emissions.
4. Although soybean would be benefitted from the future climate change, corn yield would be reduced in Eastern Canada region. Nevertheless, the N losses in drainage and GHG emissions would increase significantly in the future if no adaptation methods were taken.

7.4 Recommendations for future research

1. The RZWQM2 needs further tests for GHG and NH_3 emissions in different types of soils, and needs to be modified and tested for predicting CH_4 emissions. The soil water dynamics of DNDC should be improved.

2. Sensitivity and uncertainty analysis for RZWQM2 parametrization should be carried out to verify the key parameters in predicting GHG emissions.

3. The impact of climate change on crop production, GHG emissions, water quality and food security can be positive or negative. Future research should be focused on adaptation to the climate change and alleviation the negative impact of the changes on environment quality and crop production. For example, rising temperature results in shorter growing period and earlier maturity, which may require cultivars with longer growing season, earlier planting date or two harvests instead of one. Moreover, nitrogen uptake by crops was found to increase with the rising CO_2 concentration, thus, more nitrogen fertilization may need to be applied for the crop yield to benefit from the climate change, which leads to more N losses in water and GHG emissions. The

temperature increase in cool regions accelerated the proliferation of insect pests, and higher chances of pests and diseases might occur. Thus, more applications of pesticide and herbicide should be taken into consideration. Consequently, the pesticide leaching could also be a concern for food security.

4. The climate change impact on GHG emissions are based on model simulations. It is recommended to conduct a field or laboratory experiment under manually changed climate to verify the warming, re-distributed precipitation, enriched CO_2 concentration effects on the mechanisms of GHG emissions.

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