Comprehensive Simulation Assessment of Nitrate Mass Loading to Groundwater from Agricultural Landscapes

by

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I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners. I understand that my thesis may be made electronically available to the public.

Abstract

Nitrate contamination of groundwater underlying intensely farmed regions has become a concern in recent decades. Agricultural system models offer the ability to advance our understanding of the nitrogen transformation processes within the root zone and the associated vadose zone transport processes that provide the link from the root zone to the saturated groundwater zone. Also, models can be used to aid in the interpretation of data collected at the experimental plot scale and to support management strategies aimed at mitigating nitrate loading to groundwater. Agricultural models may represent various physical, chemical and biological processes at different levels of complexity, and their application is normally associated with uncertainties originating from different sources including parameter estimation, input data and model structure and quality. Hence, a given agricultural system must be simulated with careful attention so that credible and defendable results are generated.

The goal of this research was to evaluate the ability of agricultural system models to simulate temporal nitrate mass loading below the root zone. To tackle this evaluation effort the following research objectives were developed: (1) determine the sensitivity of key model output responses for a selected agricultural system model to the variability of input parameters over different vertical-spatial and temporal domains; (2) compare and elucidate the ability of two agricultural system models to simulate water flux and nitrate loading at the plot scale; (3) explore the capability of an agricultural system model that is fully calibrated at one location to simulate the water flux and nitrate loading at another location with similar soil and cropping characteristics; and (4) use a calibrated and validated agricultural system model to predict groundwater recharge and nitrate loading resulting from the implementation of a best management practice (BMP) established on a parcel of land where groundwater impacts due to nitrogen application have been observed.

Two study sites where elevated nitrate concentrations in groundwater have been observed were used in this research. The primary study site was the shallow unconfined Abbotsford Aquifer, located in Lower Fraser Valley, British Columbia, where

elevated groundwater nitrate concentration is attributed to excess nitrogen inputs as mineral fertilizer and poultry manure compared with the nitrogen demand of the red raspberry (*Rubus ideaus* L.) crop. The secondary study site was the Thornton Well Field in southwestern Ontario where a legacy of agricultural activities in the area (i.e., corn, soybeans, wheat and grass) has resulted in an increased nitrate concentration at the extraction wells that provide a portion of the drinking water supply for Woodstock, Ontario.

Two study fields were employed in this research at the Abbotsford Aquifer study site: (a) the Clearbrook substation experimental farm, and (b) a commercial raspberry farm located 2 km away from the experimental farm. At the Clearbrook substation, experimental plots (randomized with replicates) each received different agricultural treatments. These plots were developed as part of the Sustainable Agriculture Environmental Systems (SAGES) project. A network of passive capillary wick samplers (PCAPS) was installed at the bottom of the root zone (depth of 55 cm) to estimate water flux and nitrate loading. This research study used data collected from three treatments during January 2009 to April 2011. One of these treatments reflects the conventional grower's practice within the Abbotsford region. At the commercial raspberry farm, water flux was estimated from daily soil moisture content and pressure data collected below the root zone. Nitrate loading was estimated from water flux estimates and soil nitrate concentration measured in soil samples collected monthly.

The Thornton Well Field study site encompasses two agricultural parcels; Parcel A and Parcel B. Parcel B was managed using BMPs involving nutrient application restrictions since 2003. Previous research efforts established various locations ("recharge stations") within Parcels A and B, and estimated temporal vertical recharge and nitrate loading for 2005 and 2007. This research study used data collected from three stations within Parcel B, and two stations within Parcel A that capture dominant cropping practices and distinctive stratigraphic profiles.

A survey of existing one-dimensional nitrogen models was performed and two agricultural system models were selected based on developed criteria (e.g., suitability, technical support, complexity); the Root Zone Water Quality Model (RZWQM) and the Coupled Model (CoupModel). Although both of these models were designed to simulate complex soil hydrological and nitrogen cycle processes for cropped systems the complexity and treatment of individual components are different. Since the magnitude and timing of nitrate load is relative to the water flow from the root zone, the performance of each model to simulate both water flux and nitrate loading processes was critical; hence calibration and validation efforts focussed on these model components in a step-wise fashion. A global sensitivity analysis (Objective 1) was performed within the locally-anticipated range of RZWQM input parameters for the Clearbrook substation experimental plots to define the uncertainty associated with the simulation results. A set of calibration parameters was selected for the RZWQM based on the outcomes of this sensitivity analysis. For the CoupModel, calibration parameters were selected based on the results of a previous sensitivity analysis. Automatic optimization engines were utilized to calibrate both models to data collected from the various treatments at the Clearbrook substation. The predictive capability of the calibrated models was evaluated (Objective 2). The best performing model was applied to the data set obtained from the commercial raspberry farm to examine the transportability of a calibrated agricultural system model to a nearby location (Objective 3). The utility of the RZWQM to predict soil water content and nitrate concentration in the vadose zone, and the long-term reduction of nitrate loading to the groundwater as a result of BMP implementation in Parcel B at the Thornton Well Field study site were investigated (Objective 4). In this application, the RZWQM was calibrated to maximize the predictive capacity, and the effects of two alternative BMP scenarios on nitrate loading from Parcel A were simulated.

The results from the global sensitivity analysis showed that out of 70 RZWQM input parameters (35 hydrological parameters and 35 nitrogen cycle parameters), in general, the field capacity (soil water content at -33 kPa) in the upper 30 cm of the soil horizon had the greatest contribution ($>$ 30%) to the estimate of the water flux and evapotranspiration uncertainty. The most influential parameters affecting the simulation of soil total nitrate content, mineralization, denitrification, nitrate loading and plant nitrogen uptake were the transient coefficient of the fast to intermediate humus pool, the carbon to nitrogen ratio of the fast humus pool, the organic matter decay rate in fast humus pool, and field capacity. The correlated contribution to the model output uncertainty was $< 10\%$ for the set of parameters investigated. The selected model outputs were not sensitive to any of the macroporosity parameters (17 parameters) possibly due to the sandy texture of the soil profile. The findings from this effort were utilized in two calibration case studies to demonstrate the utility of a global sensitivity analysis to reduce the risk of over-parameterization, and to identify the vertical location of observational data that are most effective to use as the RZWQM calibration targets when water flux estimates are a key focus.

A comparison of the simulation results of the RZWQM and the CoupModel to data collected from the various treatments at the Clearbrook substation revealed that the RZWQM outperformed the CoupModel when water flux was the key model output. The superior performance of the RZWQM for predicting water flux was due to the better simulation of evapotranspiration by this model. The CoupModel, on the other hand, was able to represent the nitrate loading time series better than the RZWQM, possibly due to the flexibility of the CoupModel for modifying plant growth parameters. Overall, both models were able to approximate annual nitrogen leaching below the raspberry root zone; however, this application requires sufficient information about driving nitrogen sink/source terms including soil organic matter condition and plant nitrogen uptake. With such information, these models were found to be reliable tools to simulate nitrogen load into the groundwater.

The CoupModel that was suitably calibrated to data from the Clearbrook substation was applied to the study field on the commercial raspberry farm. Using the transported model, water flux was overestimated by 24%, and nitrate flux was simulated with an average error of 104%. When locally-measured hydraulic parameters were used in place of the calibrated hydraulic parameters, water flux simulation error remained intact, and the average nitrate flux error was reduced only by 17%

to $< 87\%$. These discrepancies between the observations and the simulations were related to the influence of the management of the raspberry inter-rows on the water and nitrate fluxes on the raspberry rows which could not be accounted in the Coup-Model one-dimensional simulation. By adopting the concept of similar media and using a single-value scaling factor method, soil hydraulic parameters were scaled to the farm level, and were used to integrate water and nitrate flux simulations across the commercial raspberry farm. The variability of soil hydraulic parameters across the field had a minimum effect on water flux simulation. The variability of soil hydraulic parameters influenced nitrate flux by up to 28% for the year in which manure was applied to the farm (i.e., when organic matter was fresh and labile), whereas for the other years of simulation, this influence was small. Therefore, transported hydraulic parameters were applicable for simulating water flow and nitrate flux (except for the year in which manure was applied) in the farm scale. It is suggested that the sandy texture of the soil profile and high precipitation rate have dominated the water and solute transport within the vadose zone, and facilitated the transportability of model regardless of the spatial variation of the soil hydraulic properties.

At the Thornton Well Field, simulated water flow and nitrate load were out of the field estimated bounds, suggesting that the simulations were associated with error. However, the performance of the calibrated RZWQM for simulating water flow and nitrate load could not be evaluated due to the uncertainties associated with the measurement techniques and calculation assumptions. According to the simulation results, post BMP annual nitrate loading was not necessarily less than the nitrate loading before BMP implementation. This was related to the complexity of the processes that affects nitrogen transformation and transport, and indicated that the effectiveness of the BMP needs to be investigated over a long time period and single field measurements cannot be used. The results from the RZWQM simulations indicate a positive agreement between post BMP nitrate loading and soil nitrate concentration, but there was no relationship between these two values.

In summary, global sensitivity analysis not only identified the most influential parameters of the model that required calibration but also provided a useful guide to define the timing and vertical-location of the observation data that is most effective to use as the calibration target, and design appropriate experiments for collecting such data. Both selected models, RZWQM and CoupModel, were reliable for prediction of nitrate loading time series below the raspberry root zone; however, the CoupModel performed better than the RZWQM due to its flexibility for modifying growth parameters when perennial crops are simulated. The calibrated CoupModel was applicable for simulating nitrate flux below the raspberry root zone in a nearby farm within the Abbotsford region except for the years when organic fertilizer was applied. While the results of this transportability effort are promising, additional validation at similar fields under different management practices is encouraged. Also, development of models that capture the effects of raspberry inter-rows cropping system on nitrate and water flux below the raspberry root zone is essential. At the Thornton Well Field, the BMPs were effective in reducing nitrate load from Parcel B farmlands into the groundwater; however, various time frames are needed to observe significant response to the BMPs at different farmlands.

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Dedication

This thesis work is dedicated to my beloved husband, Amir, who has been a constant source of support and encouragement, to the greatest influence of my life, my father, and to my mother for her constant and unconditional love.

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Chapter 1

Introduction

1.1 Nitrogen

Nitrogen contamination of groundwater has become a global environmental problem since the 1970s as a result of an increase in the application of organic and synthetic nitrogen fertilizers. Nitrate is the primary form of nitrogen leaching from agricultural land into groundwater since it is highly soluble and easily washed out of the soil profile. The risk of nitrate contamination of groundwater, in general, depends on the intensity of nitrogen fertilizer use and the vulnerability of the aquifer to leaching (Nolan et al., 1988).

High nitrate levels in drinking water pose a health risk (Health Canada, 1987). An excessive level of nitrate in drinking water causes the conversion of nitrate to nitrite in the body and reduces the oxygen-capacity of the blood stream. This condition leads to a serious and fatal illness in infants called "blue-baby syndrome" or methaemoglobinaemia (Addiscott et al., 1991). Also, some theoretical and experimental studies have shown a link between nitrate in potable water and stomach cancer (Risch et al., 1985; Dutt et al., 1987). Since aquifers are a main source of fresh water (i.e., in Canada, more than 30% of the population rely on groundwater for domestic use (Environment Canada, 2012a)), nitrate contamination of groundwater is of great concern.

1.2 Nitrogen Modeling

Many biochemical and physical processes contribute to the nitrogen cycle and the resultant nitrate leaching to the underlying aquifer. The variability and interconnectivity of these processes make nitrogen transformation and transport a complex environmental phenomenon. Quantitative synthesis of this complex is beyond brain's ability. Moreover, field evaluation of these processes under different field conditions is practically impossible and therefore, mathematical modeling has an important role to play. Due to close link between carbon cycle and nitrogen cycle, they are often simulated together in nitrogen models (Shaffer, 2002). In nitrogen models, nitrogen cycle processes are simulated as functions of environmental driving variables such as carbon and nitrogen substrates, temperature, moisture, oxygen and pH. To represent real-world conditions, nitrogen cycling processes are often connected with other components of the soil-crop system including crop growth, agricultural management, soil chemistry, and water and solute transport to generate an agricultural nitrogen model (Shaffer, 2002). Models can be used to advance our understanding of nitrogen processes and estimate responses to anthropogenic alterations (Irvine et al., 2005). Also, quantification of the impact of agricultural management on groundwater quality and supporting best management practices (BMPs) that aim at mitigating nitrate leaching is a common application of agricultural nitrogen models.

The availability and use of nitrogen models has increased rapidly since the 1970s. Based on the published literature, at least 15 well-known models, equipped with various attributes, have been developed in North America and Europe for simulating different aspects of nitrogen transformation and transport in agricultural systems (Ma and Shaffer, 2001; Malcolm et al., 2001; Wu and McGechan, 1998). Models are usually ranked according to the amount of detail they contain (Shaffer, 2002; Shaffer et al., 2001). Addiscott et al. (1991) classified the models as to whether they are functional or mechanistic, and if they were developed as a research or management tool. Mechanistic models incorporate the best classical theory of a process while simple functional models provide a general description of the phenomenon. In general, functional models belong to the management category while mechanistic models are mostly developed for research purposes. Functional models simplify processes whereas mechanistic models can be used over a wider range of conditions. The usage of functional models is often questionable because of their inherent simplifications. In contrast, mechanistic models require detailed input data and the specification of numerous parameters which is a disadvantage (de Willigen, 1991). Comparison of models is usually difficult due to their different conceptual framework (Arora and Gajri, 1996).

1.3 Model Application and Assessment

Due to the complexity of the processes involved, agricultural systems must be modeled with care (Ma and Shaffer, 2001; Grant, 2001). The applicability of models varies significantly, and the acceptance of model simulation results should be based on appropriate testing. Many studies have been conducted to evaluate the utility of nitrogen models under various conditions using laboratory and/or field data. Calibration is almost always a strategic component of model application and evaluation. With model calibration, users develop confidence that a particular model performs appropriately for a given local condition. One of the features of the recently developed agricultural models includes incorporation of more physical and biological components relevant to the farming system (Ahuja et al., 2002). With an increase in model complexity, parameter requirements grow and hence the number of parameters requiring calibration can be exceedingly large. Using traditional trial-and-error calibration approaches for such a situation is time-consuming and subjective, and hence automatic calibration or inverse modeling is an appropriate technique (Vanclooster et al., 2000; Abrahamson et al., 2005; Vassiljev, 2006). Sensitivity analysis is often coupled with calibration, and is performed during the early stages of model application. Typically, sensitivity analysis is applied to identify critical parameters of the model by illustrating the effect of given range of error or uncertainty in a parameter on the simulated results (Delleur, 2010). Following model calibration, efforts have to be made to assure that the calibrated model is valid by comparing model results with field or laboratory data. The scientific definition of model validation implies when a model representation is within some acceptable level of accuracy. However, the definition of acceptable level is almost always subjective, that is, one scientist may confirm a model as valid, whereas another may recognize the model as invalid. Validation is often recognized as historical matching of model simulations with observed data. Once a model is deemed as validated; that is, it yields credible simulation results, it can be used to develop BMPs or to evaluate its effectiveness.

It adds to the value of a calibrated model if it is shown to be transportable (i.e., be able to predict nitrate leaching in a different location than the calibrating site with relevant environmental variables). The transportability of a model depends on the level of similarity in climate conditions, soil geometry and agricultural practices that exist between the two locations. Model transportability is particularly of interest when considering the fact that nitrate is a non-point source pollutant and it often needs to be evaluated at different locations within a landscape to integrate agricultural impact on groundwater quality. Transportable models are especially useful for poor accessible areas with limited possibilities for field assessment of nitrate leaching but strong contribution to the aquifer contamination.

1.4 Research Objectives

The main purpose of this study was to assess the ability of selected agricultural nitrogen models to simulate temporal nitrate loading below the root zone under different agricultural management and environmental conditions. The findings from this study will improve our understanding of the nitrogen transformation and transport processes within the root zone and their effect on potential ground water contamination. The objectives of this study were to:

1. Determine the sensitivity of key model output responses for a selected agricultural system model,

2. Assess the ability of selected agricultural nitrogen models to simulate temporal nitrate leaching below the root zone, and investigate the reasons behind expected discrepancies in the simulated results among those models,

3. Examine the transportability of the best performing model to another location within the same physiographic region, and

4. Study the effectiveness of the BMPs that aim at mitigating nitrate loading.

1.5 Thesis Structure

The primary study site for this research was the Abbotsford Aquifer located in the Lower Fraser Valley, BC. The secondary study site was the Woodstock Well Field located near Woodstock, ON. The average nitrate concentration in both of these aquifers has exceeded the maximum allowable concentration (MAC of 10 mg $NO_3^- - N\ L^{-1}$) for more than two decades, primarily due to agricultural activities. The Woodstock Well field is mostly under the cultivation of cereals, while cultivation of berries and poultry production are the dominant activities over the Abbotsford Aquifer. The sediment profile in the Abbotsford Aquifer is homogeneous sandy gravel but the Woodstock sediment profile consists of variable soil materials with layered aquifers and aquitards. The two study sites with different soil geometries, weather conditions and agricultural management practices allowed the objectives of this research to be explored over a range of field conditions.

A survey of existing agricultural nitrogen models was performed and two models were selected based on developed criteria (e.g., suitability, technical support and complexity); the Root Zone Water Quality Model (RZWQM) and the Coupled Model (CoupModel). Although both of these models were designed to simulate complex soil hydrological and nitrogen cycle processes for cropped systems the complexity and treatment of individual components are different.

The thesis is organized into 6 chapters of which 4 are core chapters (Chapters 2 to 5) addressing the research objectives. Each chapter is written as stand-alone contribution; hence some repetition was unavoidable. This research is structured as follows:

Chapter 2 focuses on a comprehensive global sensitivity analysis that was undertaken to investigate how the RZWQM key outputs perform across the range of uncertainty associated with 70 hydrological and nitrogen cycle parameters for different vertical-spatial and temporal domains (Objective 1). The correlation of the input parameters as well as the non-linear behaviour of the model was accounted for. In this sensitivity analysis, not only the parameters' importance was ranked but also the contribution of individual input parameters to the output uncertainties was apportioned. The sensitivity analysis results were used in two case studies for performing a robust and effective calibration.

To evaluate the performance of the selected models (Objective 2), first, influential model parameters, defined from Chapter 2 for the RZWQM and from available literature for the CoupModel, were calibrated. Then, simulated results of the calibrated models were compared to the observations for model validation. The emphasis of this study was on nitrogen fate and transport processes. Since the magnitude and timing of nitrogen transport is relative to the water flow from the root zone, the performance of each model to simulate both water flux and overall nitrate loading processes was critical. Therefore, calibration and validation efforts were performed on these model components in a step-wise fashion in order to capture the processes that deliver the best estimate, and compare the models on a process-basis. This comparison and elucidation was the focus of Chapter 3.

Chapter 4 presents and discusses the results of the transportability analysis (Objective 3). In the transportability analysis, the capability of the best performing model, determined in Chapter 2, was explored to simulate the water flux and nitrate loading at another location than the calibrating site with similar soil and cropping characteristics.

Finally, the effectiveness of a long-term BMP to reduce nitrate leaching to groundwater was investigated in Chapter 5 (Objective 4). Before this investigation, the model was calibrated to maximize its predictive capacity and validated to inform about its prediction ability. The model was also used as a supporting tool to predict the impact of two hypothetical BMPs scenarios that were proposed to reduce nitrate leaching from an agricultural parcel which historically have been under conventional farming practice (non-BMP).

Chapter 6 includes a summary of important conclusions and implications emerging from this research. It also provides an overview of recommendations for future research to support nitrogen modeling, particularly with the goal of nitrate leaching assessment.

Chapter 2

Quantitative global sensitivity analysis of the RZWQM to warrant a robust and effective calibration

Outline

Sensitivity analysis is a useful tool to identify key model parameters as well as to quantify simulation errors resulting from parameter uncertainty. The Root Zone Water Quality Model (RZWQM) has been subjected to various sensitivity analyses; however, in most of these efforts a local sensitivity analysis method was implemented, the nonlinear response was neglected, and the dependency among parameters was not examined. In this study we employed a comprehensive global sensitivity analysis to quantify the contribution of 70 model input parameters (including 35 values of 21 hydrological parameters and 35 nitrogen cycle parameters) on the uncertainty of key RZWQM outputs relevant to raspberry row crops in Abbotsford, BC, Canada. Specifically, 9 model outputs that capture various vertical-spatial and temporal domains were investigated. A rank transformation method was used to account for the nonlinear behaviour of the model. The variance of the model outputs was decomposed into correlated and uncorrelated partial variances to provide insight into parameter dependency and interaction. The results showed that, in general, the field capacity (soil water content at -33 kPa (Nachabe, 1998)) in upper 30 cm of the soil horizon had the greatest contribution (>30%) to the estimate of the water flux and evapotranspiration uncertainty. The most influential parameters affecting the simulation of soil nitrate content, mineralization, denitrification, nitrate leaching and plant nitrogen uptake were the transient coefficient of fast to intermediate humus pool, the carbon to nitrogen ratio of the fast humus pool, the organic matter decay rate in fast humus pool, and field capacity. The correlated contribution to the model output uncertainty was <10% for the set of parameters investigated. The findings from this effort were utilized in two calibration case studies to demonstrate the utility of this global sensitivity analysis to reduce the risk of over-parameterization, and to identify the vertical location of observations that were the most effective to use as RZWQM calibration targets when water flux estimates are a key focus.

2.1 Introduction

Models are useful tools to evaluate the effects of agricultural activities on the environment, and to inform and support the decision making process (Ahuja et al., 2002). One of the features of the recently developed agricultural models includes incorporation of more physical and biological components of the farming system (Ahuja et al., 2002). With increasing model complexity, parameter requirement of the model grows. Uncertainty in the value of the model input parameters due to factors such as spatial variability and measurement errors is a major concern in model application. Typically, Sensitivity Analysis (SA) is applied to identify critical parameters of the model, and to apportion the output uncertainty to the uncertainty in the input parameters.

In most SA investigations, parameters are perturbed individually around their baseline values. The range of perturbation is either a fixed percentage or defined based on experimental estimates. The latter particularly answers the question of how much input parameter estimation errors or uncertainties are reflected in model outputs. The quantitative information provided by a SA can be used to improve the calibration process by reducing the number of parameters that require fitting (e.g., Spear and Hornberger (1980)). This reduces the risk of over-parameterization, which occurs when the amount of information contained in the observational data is insufficient for calibration (Jakeman and Hornberger, 1993), and hence only some of the model input parameters suffice to represent most of the information contained in the observational data. Over-parameterization can result in over-fitting and restricts model prediction accuracy (Jakeman and Hornberger, 1993; Beven, 2006). SA is a useful tool not only for identifying the important parameters that govern the object of the calibration (i.e., desired model output), but also for investigating the type, location and time of field observations that are most effective for calibration of the important parameters. For example, Shoemaker (2004) determined that dispersivity is an influential parameter for simulating hydraulic head, salinity and flow; and, through sensitivity analysis, identified the type and location of the field observations that are most effective for calibration of this parameter. It is expected that model outputs, with common influential parameters, contain information about one another, and are likely to be most effective as calibration targets when estimation of the other one is the key focus of the calibration.

SA techniques are classified into the following two groups: local SA methods, which test the model output sensitivity one parameter at a time by holding other parameters at nominal values, and global SA methods, which reflect the output sensitivity associated with the variation of all model parameters simultaneously (Saltelli and Sobol, 1995; Jacques et al., 2006). Some of the well-known global SA techniques include the Fourier amplitude sensitivity test (FAST) (Saltelli et al., 1999, 2008; Lu and Mohanty, 2001), sampling-based methods (Helton and Davis, 2002, 2003; Helton et al., 2006), analysis of variance (ANOVA) (McKay, 1997; Winter et al., 2006) and other techniques (Morris, 1991; Campolongo et al., 2007). In most SA methods, it is presumed that the model input parameters are independent; however, the correlation among input parameters can play an important role in model prediction and uncertainty (Xu and Gertner, 2008). For example, Pan et al. (2011) concluded that permeability uncertainty had the greatest contribution to the simulated percolation flux and tracer transport uncertainty when the parameters were assumed to be independent. But when parameter correlation was considered, uncertainties in the van Genuchten parameter (n) and porosity had larger contributions to the uncertainty in the model outputs.

The Root Zone Water Quality Model (RZWQM) (Ahuja et al., 2000a) is a one-dimensional model that allows the user to simulate the physical, chemical, and biological processes in the root zone, and evaluate the impact of agricultural management systems on crop productivity and environmental quality. The initial version of RZWQM was developed in 1992 in response to the lack of comprehensive models for root zone processes by a team of USDA-ARS scientists. Since then, the model has passed through various levels of improvement and assessment. In most of the SA efforts performed on the RZWQM, local approaches were used (Ahmed et al., 2007; Ma et al., 2004; Walker et al., 2000; Wu et al., 1996). Ma et al. (2000) performed a global SA (on a corn field in eastern Colorado, USA where manure was applied) on four groups of RZWQM parameters: soil physical properties (i.e., saturated hydraulic conductivity for different soil layers), organic matter nitrogen cycling, plant growth, and irrigation and manure application rates. However, only the parameters of one group were perturbed at a time, while the parameters in other groups were held at their baseline values. Ma et al. (2000) concluded that the model outputs plant N-uptake, silage yield, and nitrate leaching were most sensitive to the plant growth input parameters and manure application rates, whereas the sensitivity to saturated hydraulic conductivity (K_{sat}) at each individual soil layer was minor. In another SA conducted by Ma et al. (2007) (on a corn and corn-soybean rotation field fertilized with manure in Nashua, Iowa, USA), the effects of experimental errors in soil hydraulic property measurements on RZWQM simulations were investigated. Ma et al. (2007) adopted the same SA method (i.e., linear regression analysis) as Ma et al. (2000) in which they perturbed a few hydraulic parameters including K_{sat}, pore size distribution index, saturated water content, lateral K_{sat} and hydraulic gradient. Ma et al. (2007) concluded that yield and biomass were not sensitive to the soil hydraulic properties. Simulated tile flow and nitrogen losses in the tile flow were sensitive to the lateral K_{sat}, saturated water content and hydraulic gradient but were insensitive to K_{sat} and the pore size distribution index. In the SA performed by Ma et al. (2000, 2007), the non-linear relationships between model inputs and outputs were not considered in the linear regression analysis, and parameters were assumed to be independent. Moreover, important model input parameters such as those that describe macroporosity were excluded.

The purpose of this present study was to identify the influential (sensitive) model input parameters in their uncertainty domain on key model output responses for different vertical-spatial and temporal domains. The study condition includes raspberry crop production in the Lower Fraser Valley in southwestern British Columbia. The utility of the quantitative results of this SA was demonstrated in two calibration-evaluation case studies for reducing the risk of over parameterization and finding the most effective observation for an effective calibration. The findings of this study are expected to provide guidance toward identification of potential sources of simulation uncertainty and effective calibration of the model.

In this study, unlike previous SA conducted on the RZWQM, the non-linear behaviour of the model was captured. In addition, the dependency and interaction of the parameters were investigated. The regression-based method proposed by Xu and Gertner (2008) was used for the global SA of the RZWQM. Since this method becomes impractical for nonlinear models, a rank transformation approach was implemented to account for nonlinear relationships (Iman and Conover, 1979). In this sample-based regression-based method, the variance of an output was decomposed into partial variances contributed by the correlated variation and uncorrelated variation of a parameter.

2.2 Materials and Methods

2.2.1 Field Description

The RZWQM input data were obtained from a field experiment conducted by Kuchta (2012) to quantify nitrate leaching under different management practices for red raspberry (*Rubus ideaus* L.) production. The field site was located at Abbotsford, BC, Canada. The site was located over the Abbotsford-Sumas Aquifer; a 160-km^2 trans-boundary aquifer is located in the Lower Fraser Valley in southwestern British Columbia, Canada and northern Washington State, USA (Liebscher et al., 1992). Elevated groundwater nitrate concentrations in this aquifer were attributed primarily to excess N inputs as mineral fertilizer and poultry manure compared with crop N demand in raspberry production (Wassenaar, 1995; Zebarth et al., 1998).

The experimental field was established in 2008. The raspberry crop was grown in rows 3 m apart. A 1.2 m wide "herbicide strip", centered on the crop row, was maintained vegetation-free through herbicide applications. Weeds were controlled in the alley through regular cultivation. This study used data collected from one treatment for the time period from January 2009 to April 2011. This treatment was chosen to reflect conventional grower's practice. Fertilizer N application each spring was 100 kg N ha^{-1} as urea surface broadcast on the herbicide strip as a split application in April and May (as described by Kuchta (2012)). Drip irrigation at the crop row was applied at 714 and 796 mm during the growing seasons in 2009 and 2010, respectively. The raspberry crop has biennial canes and perennial roots and crown. Each year both first year vegetative canes (primocanes) and second year fruiting cases (floricanes) are present (Crandall, 1995).

The unconfined glacial-fluvial Abbotsford Aquifer is described as an extremely gravel-sandy texture (Mitchell et al., 2003). The surficial soil layer is well-drained due to its sandy texture. At the study site, the depth of the surficial soil at which the transition to the coarse gravelly material occurs was observed at 55 cm (Kuchta, 2012). Detailed soil horizon information at the study site is given in Table 2.1. The average annual precipitation is 1573 mm, and the average monthly temperature ranges from 2.6 °C in January to 17.7 °C in August with an annual average temperature of 10.0 °C (Environment Canada, 2012b). The required daily weather data to drive the model were obtained from a weather station located at the Abbotsford Airport which is approximately 2 km northwest of the study site (Environment Canada, 2012b). During the study period (January 2009 to April 2011), the mean monthly temperature ranged from 1 °C in December 2009 to 20.4 °C in July 2009. The annual precipitation in 2009 and 2010 was 1387 and 1495 mm.

At the study site, a network of passive capillary wick samplers (PCAPS) (Figure 2.1) was installed in the herbicide strip (Kuchta, 2012). The top of the PCAPS was located at 55 cm depth which was considered as the bottom of the root zone. The volume and nitrate concentration of the solution captured by the PCAPS were measured every 2 weeks from April 2009 to April 2011. Soil volumetric water content (θ) integrated at the 30 cm uppermost soil layer was monitored using Campbell Scientific CS616 Water Content Reflectometers (WCR) (Kuchta, 2012). Soil volumetric water content was also recorded at the depths of 38, 56 and 75 cm using 5TE sensors (Decogon Devices, 2012). For the purpose of modeling, it was assumed that at the end of the growing season 100 kg ha^{-1} crop residue was released. Also, the length of growing season was set at 240 days from March 15 to November 10 for both 2009 and 2010.

2.2.2 Sensitivity Analysis of the Root Zone Water Quality Model (RZWQM)

In this SA, 70 input parameters were investigated: 35 values of 21 hydrological parameters and 35 nitrogen cycle parameters. The testing ranges of the hydrologi-

Figure 2.1: View of PCAPS (from Kuchta (2012)).

Table 2.1: Soil horizon information based on the field survey and laboratory characterization.

Depth (cm)	Reference	Soil classification and texture	Gravel (%)	Sand (%)	Silt & Clay (%)	Soil organic matter (gr OM gr^{-1}soil)
0-25	Layer 1 (L1)	Loam	4	26	70 (6-11% clay)	0.0325
25-60	Layer 2 (L2)	Loam	5	31	64 (3-5% clay)	0.0118
60-100	Layer 3 (L3)	Sand	30	64	0	0.0164

cal parameters were determined from their uncertainty domains based on available field data and recommended and/or literature values (Table 2.2). In the RZWQM, a baseline value is recommended for each of the nitrogen cycle parameters (Table 2.3). The testing bounds of each nitrogen cycle parameter were assumed to deviate by ±20% around the recommended baseline values. A uniform distribution was assumed for each parameter in its testing domain.

2.2.2.1 Hydrological Parameters

It often happens that measured soil hydraulic properties are not available, and that the soil water retention curve (SWRC) must be estimated from simpler known properties (Ahuja et al., 2000b) such as the one-parameter Brooks and Corey method, proposed by Williams and Ahuja (1992). This simplified method was used for estimating the SWRC. This method requires θ at -0.33 kPa soil matric potential to reflect the field capacity (FC) (Nachabe, 1998). The testing ranges for soil bulk density (ρ_b), K_{sat} and FC for each soil layer were defined from the available RZWQM database, based on the soil horizon information of the upper 1 m (Table 2.1). Since there is a significant amount of humus in upper soil layers, the ρ_b ranges were justified. Also, due to the existence of a significant amount of gravel in the soil, the K_{sat} values were adjusted for gravelly soils (Smith and Mullins, 2001; Clapp and Hornberger, 1978). The bounds for silt and clay particles in Layer 1 and 2 were assigned based on soil texture (Table 2.1). The testing ranges for most of the macroporosity parameters and the non-uniform surface mixing equation constant were set according to the maximum allowable and available ranges in the RZWQM. The non-uniform surface mixing equation constant controls the amount of chemical extractions from the soil surface to the overland flow during rainfall. Extracted chemicals then either move to the macropores or run off. The range for the field saturation fraction and the total macroporosity in each soil layer were set to the values recommended in the model user's guide. The field saturation fraction represents the maximum degree of saturation that can occur when the soil is near total saturation. This has been mainly attributed to the presence of entrapped air, and the total macroporosity is defined as the volume of macropores divided by soil bulk volume. Dry soil, wet soil, crop and crop residue albedo bounds were set to recommended ranges (Ahrens et al., 2011; Oke, 1992). According to Natural Resources Canada (2012) the average percentage of daylight hours is between 30 and 40% for the Abbotsford area and this range was adopted as the average sunshine fraction.

2.2.2.2 Nitrogen Cycle Parameters

In the RZWQM, soil organic matter is partitioned into the following five computational pools based on their physical and chemical properties: fast residue pool, slow residue pool, fast humus pool, intermediate humus pool and slow humus pool. The residue pools are identified based on their composition, and the humus pools are recognized according to their half-lives. Each pool of the five pools is characterized by a specific C:N ratio (5 parameters) and a first-order decay constant (5 parameters). The fast and intermediate humus pools are recognized as mineralizable nitrogen pools. The following options exist regarding the soil organic matter in each of these pools: transfer to another pool with a specific interpool transformation coefficient (4 parameters); assimilated into three microbial biomass pools including heterotrophic decomposers, nitrifiers, and denitrifiers; and/or released as CO_2 (4 parameters). Processes such as nitrification, denitrification, volatilization and hydrolysis are simulated during these transformations with specific reaction rate coefficients (4 parameters). Both zero- and first-order rate equations are used for the nitrification process depending on the NH_4^+ concentration/activity. Denitrification, volatilization and hydrolysis are modeled as first-order processes. The three microorganism pools are characterized with their specific C:N ratios (3 parameters), and they dynamically respond to soil environmental factors such as soil oxygen content (1 parameter), water content and temperature. During the nitrogen cycle, CO_2 and CH_4 are used as a source/sink for carbon to maintain C:N ratios constant in all pools. The assimilation of carbon into biomass pools is not modeled with state equations specific to microbial growth, but rather is estimated from the

Table 2.2: Testing range of selected soil hydrological parameters for the SA. L1, L2 and L3 denote soil Layers 1 to 3, respectively.

		Parameter	Unit	Testing range	Comments
1	physical parameters	ρ_b - L1	g cm^{-3}	1.00-1.42	loam soil containing significant humus
2		ρ_b - L2	g cm^{-3}	1.13-1.42	loam soil containing less humus but more sand and gravel than upper soil layer
3		ρ_b - L3	g cm^{-3}	1.49-2.00	medium sand with gravel
4		Soil clay fraction - L1	%	6-11	silt: 60-65%
5		Soil clay fraction - L2	%	3-5	silt: 59-61%
6	Hydraulic parameters	K_{sat} - L1	cm hr^{-1}	1.3-8.3	based on RZWQM database adjusted for coarser materials(1),(2)
7		K_{sat} - L2	cm hr^{-1}	1.3-8.3	based on RZWQM database adjusted for coarser materials(1),(2)
8		K_{sat} - L3	cm hr^{-1}	21.0-81.4	based on RZWQM database adjusted for coarser materials(1),(2)
9		FC - L1	m^{3}m^{-3}	0.2-0.3	based on RZWQM database
10		FC - L2	m^{3}m^{-3}	0.2-0.3	based on RZWQM database
11		FC - L3	m^{3}m^{-3}	0.02-0.10	based on RZWQM database
12	Macroporosity parameters	Sorptivity factor for lateral infiltration	–	0-1	maximum allowable range by RZWQM
13		Macropore express fraction	–	0-1	maximum allowable range by RZWQM
14		Effective lateral infiltration wetting thickness (radial holes)	cm	0.01-2	maximum allowable range by RZWQM
15		Effective lateral infiltration wetting thickness (cracks)	cm	0.01-2	maximum allowable range by RZWQM
16		Total macroporosity - L1	m^{3}m^{-3}	0-0.001	recommended range by RZWQM: 0 to 0.1% of soil bulk volume
17		Total macroporosity - L2	m^{3}m^{-3}	0-0.001	recommended range by RZWQM: 0 to 0.1% of soil bulk volume
18		Total macroporosity - L3	m^{3}m^{-3}	0-0.001	recommended range by RZWQM: 0 to 0.1% of soil bulk volume
19		Average radius of cylindrical pores-L1	cm	0.001-1	maximum allowable range by RZWQM
20		Width of rectangular cracks - L2	cm	0.001-1	maximum allowable range by RZWQM
21		Width of rectangular cracks - L3	cm	0.001-1	maximum allowable range by RZWQM
22		Length of cracks in lower - L2	cm	0-10	maximum allowable range by RZWQM
23		Length of cracks in lower - L3	cm	0-10	maximum allowable range by RZWQM
24		Average length of aggregate - L2	cm	0-10	maximum allowable range by RZWQM
25		Average length of aggregate - L3	cm	0-10	maximum allowable range by RZWQM
26		Fraction of dead end pores - L1	–	0-1	maximum allowable range by RZWQM
27		Fraction of dead end pores - L2	–	0-1	maximum allowable range by RZWQM
28		Fraction of dead end pores - L3	–	0-1	maximum allowable range by RZWQM
29	Other parameters	Field saturation fraction	–	0.8-1.0	recommended range by RZWQM: 0.8-1
30		Non-uniform mixing equation constant	cm^{-1}	0-100	maximum allowable range by RZWQM
31		Albedo of the dry soil	–	0.15-0.33(3)	
32		Albedo of the wet soil	–	0.05-0.15(3)	
33		Albedo of the crop at maturity	–	0.15-0.30(3)	
34		Albedo of fresh residue	–	0.35-0.60(3)	
35		Average daily sunshine fraction	–	0.30-0.40(4)	

(1) Smith and Mullins (2001); (2) Clapp and Hornberger (1978); (3) Ahrens et al. (2011) and Oke (1992); (4) Natural Resources Canada (2012)

Table 2.3: Baseline value and ranges of selected nitrogen cycle parameters.

		Parameter	Unit	Baseline	±20% deviation
1	C:N Ratio	Slow residue pool	–	8	6.4-9.6
2		Fast residue pool	–	80	64-96
3		Fast humus pool	–	8	6.4-9.6
4		Intermediate humus pool	–	10	8-12
5		Slow humus pool	–	11	8.8-13.2
6		Aerobic heterotrophs (decomposers)	–	8	6.4-9.6
7		Autotrophs (nitrifiers)	–	8	6.4-9.6
8		Anaerobic heterotrophs (denitrifiers)	–	8	6.4-9.6
9	Transformation coefficient	Slow residue pool to Intermediate humus pool	–	0.3	0.24-0.36
10		Fast residue pool to Fast humus pool	–	0.6	0.48-0.72
11		Fast humus pool to Intermediate humus pool	–	0.6	0.48-0.72
12		Intermediate humus pool to Slow humus pool	–	0.7	0.56-0.84
13	Organic matter decay coefficient	Slow residue pool	s day^{-1}	1.67E-07	1.34E-07-2.01E-07
14		Fast residue pool	s day^{-1}	8.14E-06	6.51E-06-9.77E-06
15		Fast humus pool	s day^{-1}	2.50E-07	2.00E-07-3.00E-07
16		Intermediate humus pool	s day^{-1}	5.00E-08	4.00E-08-6.00E-08
17		Slow humus pool	s day^{-1}	4.50E-10	3.60E-10-5.40E-10
18	Reaction rate coefficient	NH_3 Volatilization	s day^{-1}	1000	800-1200
19		Nitrification	s day^{-1}	1.00E-09	8.00E-10-1.20E-09
20		Denitrification	s day^{-1}	1.00E-13	8.00E-14-1.20E-13
21		Hydrolysis of urea	s day^{-1}	2.50E-4	2.00E-04-3.00E-04
22	Activation energy coefficient	Aerobic heterotrophs (decomposers)	–	88.6	70.88-106.32
23		Autotrophs (nitrifiers)	–	61	48.80-73.20
24		Anaerobic heterotrophs (denitrifiers)	–	63.1	50.48-75.72
25		Oxygen limitation	–	0.05	0.04-0.06
26	Assimilation factor	Converting decayed OM to assimilated biomass	–	0.267	0.214-0.320
27		Converting nitrified NH_4^+ to Autotroph biomass	–	0.010	0.008-0.012
28		Efficiency factor for denitrifiers nitrogen uptake	–	0.133	0.106-0.160
29		Denitrification rate converting to anaerobic OM decay rate	–	0.10	0.08-0.12
30	Population conversion factor	Aerobic heterotrophs (decomposers)	#orgs g^{-1}soil	950	760-1140
31		Autotrophs (nitrifiers)	#orgs g^{-1}soil	9500	7600-11400
32		Anaerobic heterotrophs (denitrifiers)	#orgs g^{-1}soil	9500	7600-11400
33	Death rate coefficient	Aerobic heterotrophs (decomposers)	s day^{-1}	5.00E-035	4.00E-35-6.00E-35
34		Autotrophs (nitrifiers)	s day^{-1}	4.77E-40	3.82E-40-5.72E-40
35		Anaerobic heterotrophs (denitrifiers)	s day^{-1}	3.40E-33	2.72E-33-4.08E-33

associated rates of reactions. The microbial death rates are proportional to their biomass (3 parameters) and calculated as a first-order process. A more detailed description of nitrogen cycle processes is discussed elsewhere (Shaffer et al., 2000).

2.2.3 Model Outputs

The SA was conducted on nine model output responses:

- water flux [cm day^{-1}],
- actual evapotranspiration ET [cm day^{-1}],
- total $NO_3^- - N$ in the 1 m soil profile [kg ha^{-1}],
- mineralization [kg ha^{-1}],
- denitrification loss [kg ha^{-1}],
- $NO_3^- - N$ leaching [kg ha^{-1}],
- plant N-uptake [kg ha^{-1}],
- θ [m^{3}m^{-3}], and
- soil $NO_3^- - N$ concentration [μg g^{-1}].

Each of these model outputs is of practical importance. Denitrification loss and $NO_3^- - N$ leaching define nitrogen losses. Water flux and ET together with nitrate concentration control the potential for nitrate leaching. Plant N-uptake is the indicators of crop growth. Mineralization is considered a source of nitrogen for plant N-uptake and nitrate leaching. Soil water content (θ) and $NO_3^- - N$ concentration are often used as the observation data to calibrate soil hydraulic and nitrogen cycle parameters (e.g., Nolan et al. (2010); Fang et al. (2010); Schmied et al. (2000); Hanson et al. (1999)). Therefore, it is necessary to determine which of the 70 model input parameters are influential and can be successfully calibrated by using the selected observations.

The seasonal influence of each parameter on seven of the nine model outputs (water flux, ET, total $NO_3^- - N$ in the soil profile, mineralization, denitrification loss, $NO_3^- - N$ leaching and N-uptake) was investigated. That is, the SA was performed separately on the accumulation of each of these outputs during two growing seasons (March - October in 2009 and 2010) and two wet/cold seasons (November - February in 2010 and 2011). Monthly precipitation and mean temperature during the growing seasons and wet/cold seasons are presented in Appendix 1. The sensitivity of each parameter on the remaining two model outputs (θ and soil $NO_3^- - N$ concentration) was investigated in winter, spring, summer and fall for both 2009 and 2010. To represent the temporal conditions, each of these outputs were averaged over seven days (the 15^{th} to 22^{nd} of January, April, July and October representing winter, spring, summer and fall, respectively) in 2009 and 2010. This averaging process smoothed out extreme environmental conditions, such as heavy rainfall, which may skew the findings. For θ content and soil $NO_3^- - N$ concentration outputs, the SA was performed at four discrete depths within the soil profile: 0-30 (averaged), 45, 60 and 85 cm. The 0-30 cm depth, for which an averaged θ was recorded in the field, covers the top soil layer (Layer 1). The 45 and 85 cm depths are located near the middle of Layers 2 and 3, respectively, and the 60 cm depth is between Layers 2 and 3, and locates 5 cm below the PCAPS lid. The purpose of this spatial discretization was to define influential parameters at various depths in the soil profile that may affect calibration.

2.2.4 Sensitivity Analysis Method

The Latin Hypercube Sampling (LHS) method was used to generate m random values ($m = 500$) for each model input parameter. A vector of m output variables ($y_1...y_k$ for $k = 1...m$) was generated by using the RZWQM for each set of random input variables ($x_1, ..., x_i$ for $i = 1...n$ where n is the number of input parameters). In this study n is 70 and is comprised of 35 values of 21 hydrological parameters and 35 nitrogen cycle parameters. If the effect of each parameter (x_i) is linear, a regression model relating each model output to the input parameters can be written as:

$$y_k = \alpha_0 + \sum_{i=1}^{n} \alpha_i x_{ik} + \varepsilon_k \tag{2.1}$$

and

$$\hat{y}_k = \alpha_0 + \sum_{i=1}^{n} \alpha_i x_{ik} \tag{2.2}$$

where $\alpha_0 ... \alpha_i$ are regression coefficients, $\hat{y}_k$ is the estimation of output, y_k as generated by the regression model and ε_k is error. For linear regression analysis, the multiple coefficient of determination, ${R_y}^2$ is given by:

$${R_y}^2 = \sum_{k=1}^{m} (\hat{y}_k - \bar{y})^2 / \sum_{k=1}^{m} (y_k - \bar{y})^2 \tag{2.3}$$

where $\bar{y}$ is the mean of the output, y_k over m realizations. If ${R_y}^2 \geq 0.7$ then the linear regression analysis is generally considered to be applicable for a SA (Saltelli et al., 2006; Manache and Melching, 2008). However, linear regression is not typically an acceptable estimator for complex models. For these cases, the rank transformation technique is implemented (Saltelli and Sobol, 1995). With this technique, the original space (raw data) of the input and output is transformed into to their ranks (i.e., rank 1 is assigned to the smallest input and output value), and the regression analysis is conducted on the ranked space with no additional computational burden. In this study, the ${R_y}^2$ value of the original space of each model output investigated was calculated, and the rank transformation was applied only when ${R_y}^2 < 0.7$. The reliability of the linear regression analysis was also tested for the ranked data before SA application.

For the decomposition method that was proposed by Xu and Gertner (2008), the model output variance associated with parameter i (V_i) was decomposed into a partial variance contributed by the uncorrelated variation (V_i^u) and the correlated variation (V_i^c) of each model input so that

$$V_i = V_i^u + V_i^c \tag{2.4}$$

If the effect of parameter x_i on the model output is approximately linear, the partial variance of y contributed by x_i can be derived from:

$$\hat{V}_i = \frac{1}{m-1}\sum_{k=1}^{m}(\hat{y}_k^{(i)} - \bar{y})^2 \tag{2.5}$$

with

$$\hat{y}_k^{(i)} = \eta_0 + \eta_i x_{ik} \quad k = \{1, ..., m\}, \;\; i = \{1, ..., n\} \tag{2.6}$$

where $\hat{y}_k^{(i)}$ is the regression estimation of output y_k by Eq.(2.6), and $\eta_0 ... \eta_i$ are coefficients from the bivariate regression between y and x_i.

The partial variance contributed by the uncorrelated variation of x_i, $\hat{V}_i^u$ can be derived from:

$$\hat{V}_i^u = \frac{1}{m-1}\sum_{k=1}^{m}(\hat{y}_k^{(-i)} - \bar{y})^2 \tag{2.7}$$

with

$$\hat{y}_k^{(-i)} = \lambda_0 + \lambda_i \hat{z}_{ik} \quad k = \{1, ..., m\}, \;\; i = \{1, ..., n\} \tag{2.8}$$

where

$$\hat{z}_{ik} = x_{ik} - \hat{x}_{ik} \tag{2.9}$$

and

$$\hat{x}_{ik} = \delta_0 + \sum_{t=1,t\neq i}^{n} \delta_t x_{tk} \tag{2.10}$$

where $\hat{y}_k^{(-i)}$ is the bivariate regression estimate of output y_k by Eq.(2.8), and $\hat{x}_{ik}$ is the regression of x_{ik} over all parameters except x_i, and $\lambda_0 ... \lambda_i$ and $\delta_0 ... \delta_t$ are regression coefficients. Based on Eq.(2.4), the partial variance contributed by the variation of x_i correlated with $x_1, ..., x_{i-1}, x_{i+1}, ..., x_n$ can be estimated by:

$$\hat{V}_i^c = \hat{V}_i - \hat{V}_i^u \tag{2.11}$$

The total variance of y, V is calculated by:

$$V = \frac{1}{m-1} \sum_{k=1}^{m} (y_k - \bar{y})^2 \tag{2.12}$$

Finally, by using the ratio of partial variances and total variance, the total (S_i), uncorrelated (S_i^u), and correlated (S_i^c) partial sensitivity indices of parameter x_i can be described by:

$$S_i = \frac{\hat{V}_i}{V} \tag{2.13}$$

$$S_i^u = \frac{\hat{V}_i^u}{V} \tag{2.14}$$

$$S_i^c = \frac{\hat{V}_i^c}{V} \tag{2.15}$$

The correlated sensitivity index of each parameter (S_i^c) quantifies the uncertainty that is contributed by that parameter due to its correlation with other parameters.

S_i^c can be negative or positive, but it is treated as positive; that is, larger $|S_i^c|$ values suggest greater sensitivity. S_i^c is negative when the correlation of a parameter with other parameters is negative.

2.3 Results and Discussion

2.3.1 Robustness of the SA Method

To determine whether the 500 sample size have converged to an acceptable degree, results from three independent sets of random data (i.e., 3 different sets or trials of 500 random values for each input model parameter) were investigated. For all model outputs, the parameters with >10% contribution to the total uncertainty, presented in all three trials with similar fractions relative to the total variance. For example, the total sensitivity indices for $NO_3^- - N$ leaching in the wet/cold Season 1 is shown in Figure 2.2a. The most influential parameters to $NO_3^- - N$ leaching uncertainty (including *FC* in Layer 1; C:N ratio of the fast humus pool; transition coefficient of fast to intermediate and intermediate to slow humus pool; OM decay of the fast humus pool; and population conversion factor of aerobic heterotrophs) were present in similar proportions in all three trials. Some parameters with a minor contribution to the uncertainty emerged in one or two trials (e.g., *FC* in Layer 3 with 4% total contribution in Trial 3) but these were relatively small compared with the other influential parameters. Similarly in Figure 2.2b, the total sensitivity indices of the influential parameters on θ at 85 cm depth in summer are shown for the three trials. The bulk density (ρ_b) and *FC* for Layer 1 and Layer 3 were the most important parameters that emerged in all trials with relatively similar importance. It was determined that the difference between the means of paired observations is not statistically significant (level of significance of 5%); however, since the number of observations was small the conclusion that the results from this SA method were robust is tentative.

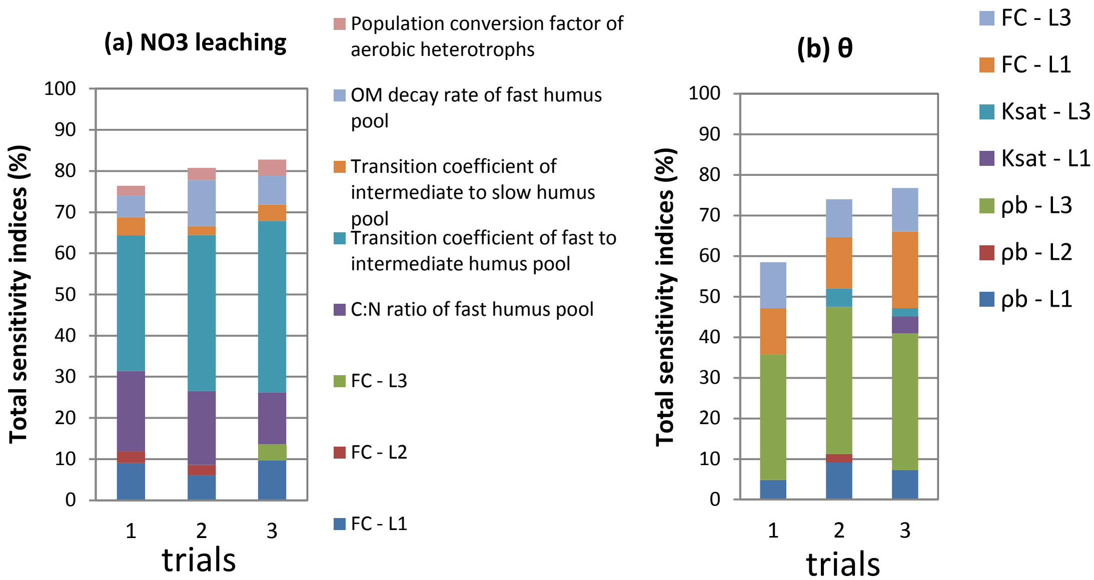

Figure 2.2: Total sensitivity indices of the influential parameters on (a) $NO_3^- - N$ leaching in the wet/cold season 1, and (b) θ at the depth of 85 cm in summer 2009, for three independent trials. L1, L2 and L3 denote Layers 1 to 3, respectively.

2.3.2 Linearity and Rank Transformation

The coefficient of determination, ${R_y}^2$ was calculated to test the reliability of the linear regression analysis for each of the model outputs. The ${R_y}^2$ values of θ for all seasons and depths were $\geq$0.7. The results of the linearity test for other output responses were variable. Rank transformation was applied for the output responses with ${R_y}^2$<0.7. This improved the ${R_y}^2$ value of most of these outputs. Model outputs with ${R_y}^2$<0.7 for both the original and ranked-transformed spaces (including water flux in the second wet/cold season and denitrification loss in the first wet/cold season) were excluded from this SA.

2.3.3 Sensitivity Analysis of the Model Outputs

2.3.3.1 Total Variance

We considered only the results of parameters with >2% contribution to the model output uncertainty since lower values are subject to numerical error (Xu and Gertner, 2008). SA results were averaged over the three trials.

The *FC* in Layer 1 was the most influential parameter for both water flux and ET in all seasons (Figure 2.3). This can be explained by the fact that *FC* is one of the only two input parameters used when one-parameter Brooks-Corey method is implemented in RZWQM simulation. In this method, *FC* defines some important soil hydraulic parameters including air-entry water suction and pore size distribution index. Subsequently, ρ_b for Layer 1 and *FC* for Layer 3 (26% and 12%, respectively) had the greatest contribution to water flux uncertainty in the wet/cold season 1. The crop albedo (14% and 24% in growing season 1 and 2) and ρ_b for Layer 1 (14% and 10% in growing season 1 and 2) were the next most influential parameters to water flux uncertainty. The contribution of *FC* in Layer 3 to water flux uncertainty during the wet/cold season 1 (12%) was smaller than the contribution of albedo of the crop in both growing seasons (14% and 24%); however, since most groundwater recharge takes place in the wet/cold season (for example, average water flux from the bottom of the root zone measured using PCAPS was 63 cm during November to April versus 26 cm during May to October for the study period starting from April 2008 to April 2010), the importance of the contributory parameters in this period of time was greater. The 20% variation of the nitrogen parameters influenced total soil nitrogen content and plant N-uptake; however, this variation did not influence the ET and water flux estimates. This is related to the lack of dependence between crop water uptake and ET, and the nutrient processes (including nitrogen processes) when woody species (raspberries in this study) are simulated in the RZWQM. That is, influences of water and nitrogen on plant processes are not independent and they often interact (Wu and Kersebaum, 2008). Water uptake is reduced under nitrogen deficit as a result of reduced root

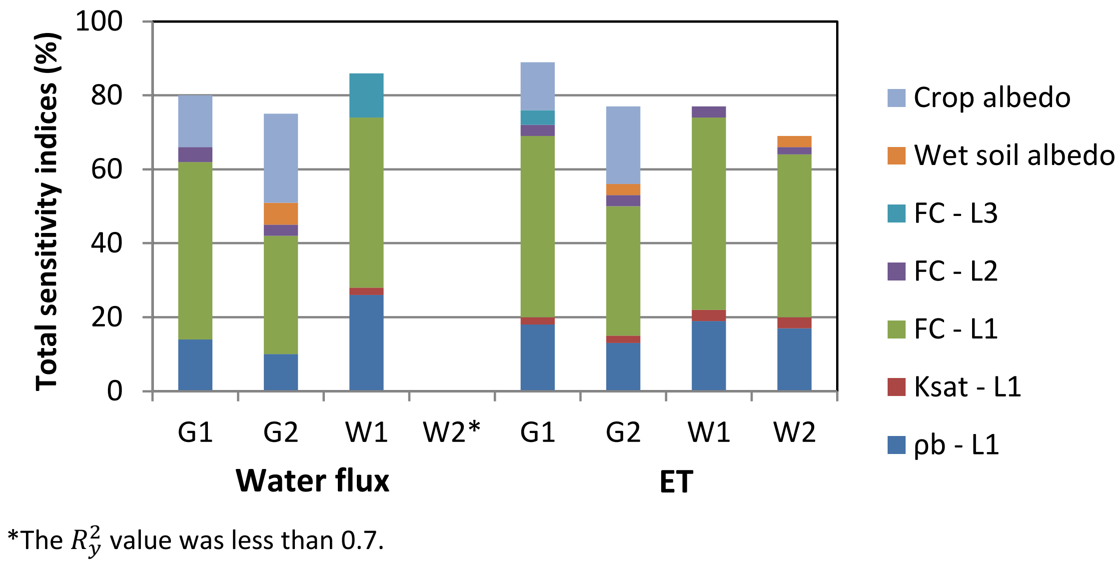

Figure 2.3: Total sensitivity indices of the influential parameters on water flux and evapotranspiration (ET). L1, L2 and L3 denote soil Layers 1 to 3, respectively. The ${R_y}^2$ value represents the multiple coefficient of determination. G1 and G2 denote growing season 1 and 2 whereas W1 and W2 represent wet/cold season 1 and 2, respectively.

hydraulic conductivity, leaf water potential and leaf area development (Radin and Boyer, 1982). Hence soil water budget and water flux is affected by nitrogen deficit.

Parameters with more than 10% contribution to the nitrogen related outputs (including total $NO_3^- - N$ in the soil profile, mineralization, denitrification loss, $NO_3^- - N$ leaching and N-uptake) are shown in Figure 2.4. The transient coefficient of fast to intermediate humus pool; C:N ratio of the fast humus pool; OM decay rate of fast humus pool; and FC in Layer 3 had the greatest contribution to these nitrogen-related model outputs.

The most influential parameter on θ at the 0-30 cm depth was FC in Layer 1, while at the depths of 45 cm and 60 cm it was FC in Layer 3, and at the depth of 85 cm it was the ρ_b for Layer 3 (Figure 2.5). This indicates that FC contributes significantly to the uncertainty in θ in the surface soils (i.e., 0-30 cm, 45 cm and 60 cm), but its importance compared with the contribution of ρ_b in the sand and

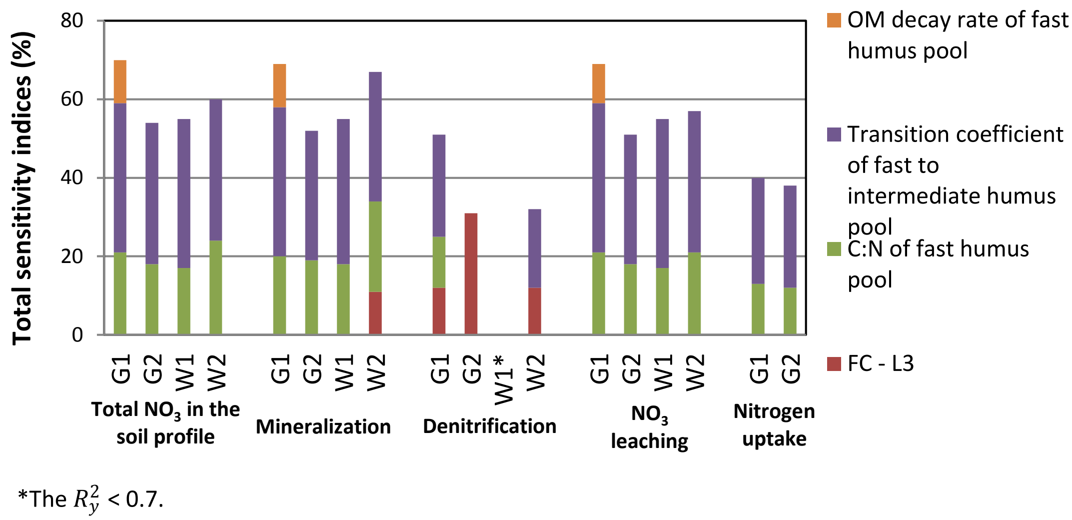

Figure 2.4: Total sensitivity indices of the influential parameters with >10% contribution to the uncertainty of model outputs: total $NO_3^- - N$ in the soil profile, mineralization, denitrification, $NO_3^- - N$ leaching and plant N-uptake. The ${R_y}^2$ value represents the multiple coefficient of determination. L1, L2 and L3 denote Layers 1 to 3, respectively. G1 and G2 denote growing season 1 and 2 whereas W1 and W2 represent wet/cold season 1 and 2, respectively.

gravel in Layer 3 was negligible at 85 cm. In general, the sensitivity of θ to different parameters did not change with different seasons (i.e., winter, spring, summer and fall), but rather was related to the physical characteristics of each soil horizon.

From the 35 nitrogen cycle parameters investigated in this study, the transient coefficient for the fast to intermediate humus pool and the C:N ratio for the fast humus pool were the most important parameters affecting the soil $NO_3^- - N$ concentration simulation uncertainty for all depths and seasons (Figure 2.6). With an average 30% contribution to the total uncertainty, ρ_b for Layer 3 was considered an influential parameter for the soil $NO_3^- - N$ concentration at the depth of 85 cm in winter, spring and summer. The average contribution of soil hydraulic parameters on the soil $NO_3^- - N$ concentration uncertainty at the depth of 85 cm (37%) , unlike the other investigated depths, was greater than the average contribution of nitrogen cycle parameters (29%), suggesting that soil $NO_3^- - N$ concentration

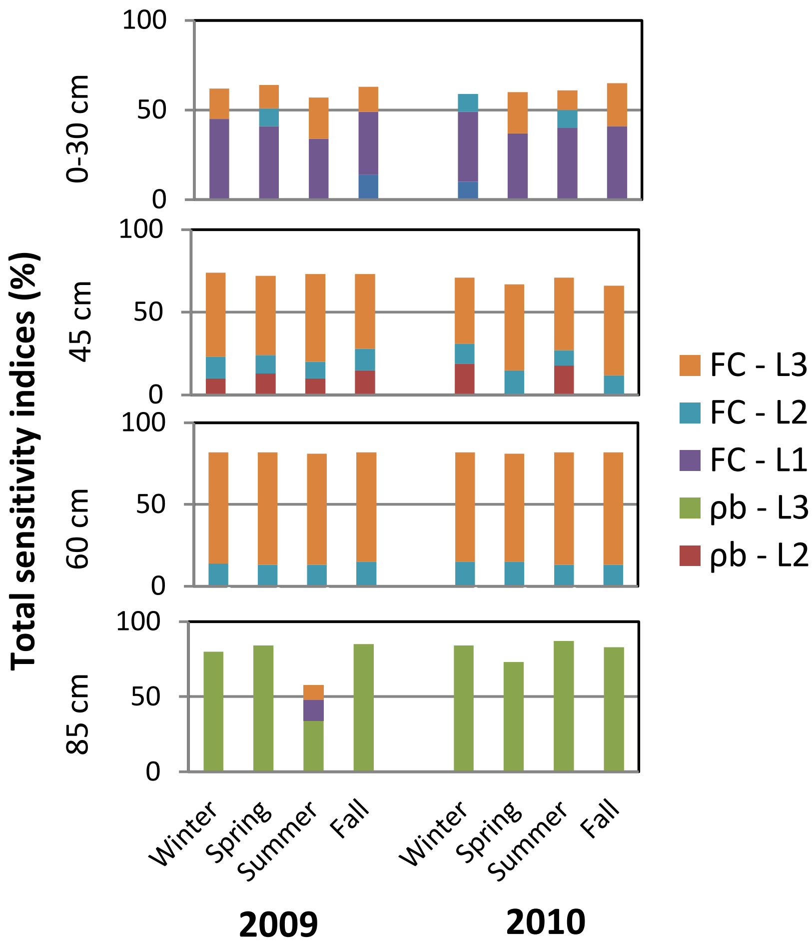

Figure 2.5: Total sensitivity indices of the parameters with more than 10% contribution to θ simulation uncertainty. L1, L2 and L3 denote Layers 1 to 3, respectively.

at this depth was more affected by the nitrogen transport processes rather than nitrogen transformation processes.

The sensitivity of model outputs to parameters varies between the growing season and the wet/cold season at this study site. Crop albedo, for example, had a significant total variance contribution to the water flux (14% and 24% in growing season 1 and 2, respectively) and ET uncertainty (13% and 21% in growing season 1 and 2, respectively), but its contribution in the wet/cold season was negligible. In contrast, the *FC* for Layer 3 was an influential parameter on water flux in the

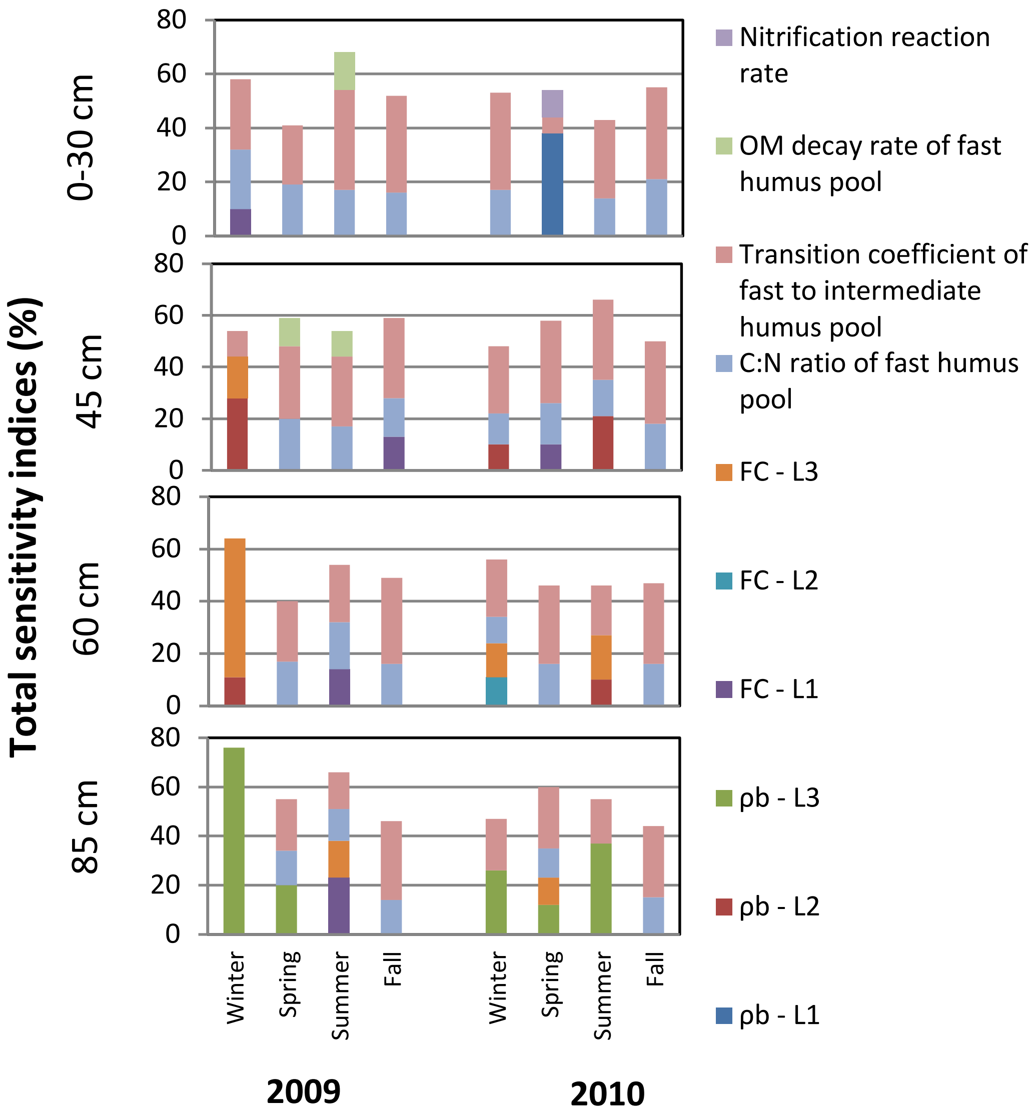

Figure 2.6: Total sensitivity indices of parameters with more than 10% contribution to soil $NO_3^- - N$ concentration uncertainty. L1, L2 and L3 denote Layers 1 to 3, respectively.

wet/cold season 1 (12%), but it has no influence to water flux uncertainty in the growing seasons. This observation needs to be considered when an output is to be investigated in a specific time/season of the year.

It was also observed that almost none of the 70 input parameters studied had the same variance contribution to one model output across similar periods of time (seasons). For some parameters this difference was high. The transition coefficient of fast to intermediate humus pool, for example, had a 26% contribution to denitrification loss uncertainty in the first growing season, while its influence in the second growing season was less than 10%. This is presumed to be a result of differences in driving factors such as weather conditions and irrigation amount/timing that vary from one year to another. These factors affect the importance of a parameter on model output uncertainties and indicate that the results from this SA are subject to different environmental and management factors.

All of the investigated model outputs were insensitive to the silt and clay fractions. This insensitivity was likely due to the narrow uncertainty ranges of the silt and clay fractions that were defined according to the site specific soil characterization. In addition, all of the tested model output responses were insensitive to maroporosity parameters. One possible reason for this result is the presence of a significant amount of sand in all soil layers (especially Layer 3) and thus matrix flow controls both water and nitrate fluxes (Köhne et al., 2009). The RZWQM uses the "gravity preferential model" which assumes that flow in the preferential domain is controlled only by gravity and is always directed downward. This flow model, however, only fits to the soils with heavy clay soils with notable cracks (Köhne et al., 2009).

2.3.3.2 Correlated Variance

Due to the possibility of numerical error, we considered only the correlated variances that had absolute values >2% (Xu and Gertner, 2008). The absolute correlated contributions (averaged over the three trials performed) of ρ_b and FC in Layer 1 on water flux and ET uncertainties were between 2 and 8% in all seasons. This magnitude was not significant compared with the total contribution of all parameters on these model outputs uncertainties (between 70 and 90%). The absolute averaged correlated contribution of influential parameters to the uncertainty of the nitrogen-related outputs (including soil $NO_3^- - N$ content, total $NO_3^- - N$ in the soil profile, mineralization, denitrification, $NO_3^- - N$ leaching and plant N-uptake) for all depths and seasons was <10%. Therefore, it can be concluded that the correlated contributions of the studied parameters on these outputs were not high. However, for some parameters, these minor correlated contributions may be considerable when studied against their total contribution. For example, the total and correlated contributions of the transition coefficient for intermediate to slow residue pool to the uncertainty of total $NO_3^- - N$ in the soil profile in the second growing season were 5 and 2%, respectively. This implies that almost 40% of the contribution of transition coefficient of intermediate to slow residue pool to this output was related to the correlation of this parameter with others. The absolute correlated contribution of most of the influential parameters on θ, for all depths and seasons, was small (i.e., 48 and 35% of the important parameters had 2-5% and 5-10% correlated index), except for the correlated contribution of ρ_b for Layer 3 for the depth of 85 cm which was approximately 14% for all seasons except for Summer 2009.

2.3.4 Calibration and evaluation

To illustrate the utility of this global SA effort, the findings were utilized in two case studies. In Case Study 1, the risk of over-parameterization and over-fitting when an excessive numbers of parameters are utilized for calibration was explored. In Case Study 2, the SA results were used to focus the selection of appropriate field observations required for effective model calibration.

Case Study 1. Over-parameterization

The RZWQM was calibrated to a data set collected from April 2009 to April 2010 at the experimental field (Kuchta, 2012). The purpose of this calibration exercise was to improve the ability of the model to predict water flux at the depth of 60 cm; therefore, the calibrating parameters were primarily selected based on the SA results for water flux output. Three calibration scenarios were investigated:

- Scenario 1(a) - All 35 hydrological parameters listed in Table 2.2 were involved in the calibration process.
- Scenario 1(b) - All influential parameters with >2% contribution to the water flux uncertainty in all seasons (Figure 2.3) were involved in the calibration process. This included seven parameters: ρ_b for Soil Layer 1; K_{sat} for Soil Layer 1; FC for Soil Layers 1, 2 and 3; and crop and wet soil albedos.
- Scenario 1(c) - The most influential parameters with >10% contribution to the water flux uncertainty in all seasons were selected (Figure 2.3), and involved in the calibration process. This included four parameters: ρ_b for Soil Layer 1, FC for Soil Layers 1 and 3, and the crop albedo.

In each calibration scenario, the field observation records from April 2009 to April 2010 comprised of both the water flux (at 60 cm depth) and θ (average over the upper 30 cm of the soil profile) were employed as calibration targets. The average contribution of the calibrated parameters to the water flux estimate uncertainty were 83, 83 and 80%, and to the θ estimate uncertainty were 80, 71 and 68%, for Scenarios 1(a), 1(b) and 1(c), respectively. For each scenario, the simulation results using the calibrated parameters were then compared with a subsequent field data set collected from April 2010 to April 2011.

The dynamically dimensioned search (DDS) global optimization algorithm developed by Tolson and Shoemaker (2007) with 8 trials (different random starting points) was used as the calibration engine. To ensure an equitable comparison based on computational requirements, 750 model evaluations where used for Scenario 1(a), and only 250 model evaluations where used for Scenarios 1(b) and 1(c). The SA method used 500 model evaluations to generate results that were then used to inform the decisions made for Scenarios 1(b) and 1(c) hence fewer model evaluations are expected. The goodness-of-fit measure used was the standard root mean square error (RMSE) objective function expressed as:

$$RMSE = \sqrt{\frac{1}{m}\sum_{i=1}^{m}(O_{WF,i} - S_{WF,i})^2} + \sqrt{\frac{1}{n}\sum_{j=1}^{n}(O_{\theta,j} - S_{\theta,j})^2} \tag{2.16}$$

where WF is the water flux (cm), θ is volumetric soil water content (%), m is the number of water flux observations, n is the number of θ observations, O represents observed values, S represents simulated values, i is the i^{th} water flux observation and j is the j^{th} θ observation. In this multi-criteria objective function, the magnitude of the two RMSE error terms is comparable over a range of parameter combinations and all observations were assigned the same relative observation weighting.

The results of the calibration and evaluation efforts for the three scenarios are presented in Figure 2.7. Bulk calibration measures for Scenario 1(a) (average RMSE of 4.02) outperformed Scenario 1(b) (average RMSE of 5.46) and Scenario 1(c) (average RMSE of 5.55) for the calibration period. The better performance for Scenario 1(a) was likely a result of the minor correlation that exists among soil hydraulic parameters, and that the set of influential parameters calibrated in Scenario 1(b) and Scenario 1(c) accounts for about 80% of the uncertainty in both water flux and soil moisture.

Scenario 1(a) calibrated parameter set performed rather poorly over the evaluation period for 2 trials as compared to parameter sets produced from Scenario 1(b) and 1(c) (Figure 2.7). As a result, on average, Scenario 1(a) yielded an average RMSE of 5.25, compared with an average RMSE of 4.87 and 4.68 for Scenarios 1(b) and 1(c), respectively. The plausible explanation for this occurrence is over-fitting due to the incorporation of an excessive number of parameters into the Scenario 1(a)

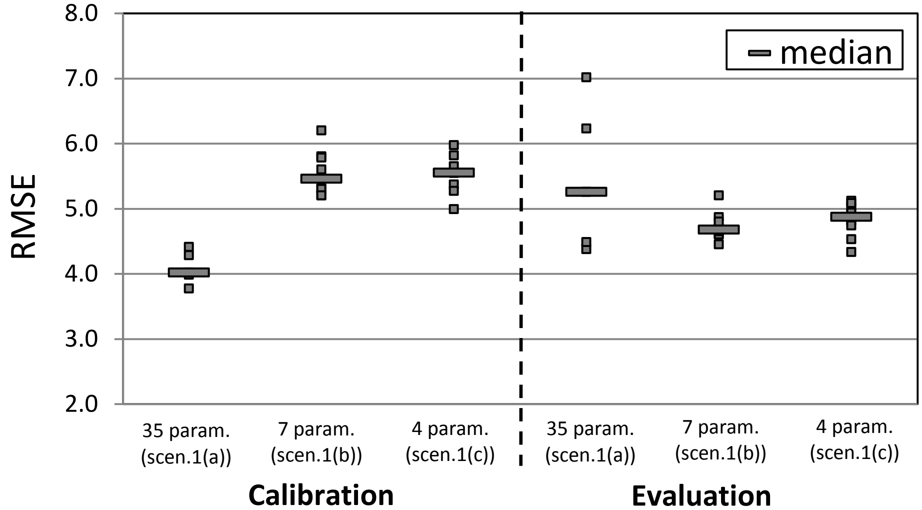

Figure 2.7: Comparison of model performances, calibrated in Case Study 1. The RMSE represents both water flux and θ estimations. Three calibrating scenarios were investigated: Scenario 1(a), all hydrological parameters were calibrated; Scenario 1(b), all influential parameters (total sensitivity index >2%) were calibrated; and Scenario 1(c), only the most influential parameters (total sensitivity index >10%) were calibrated. The default parameters included the baseline values of the calibrated parameters. Eight calibration trials were performed for each scenario. Three of the eight calibration trials for Scenario 1(a) failed to converge.

calibration. The performance of Scenario 1(b) and Scenario 1(c) were essentially identical suggesting that the four most influential parameters that were identified in the SA actually control the variation of the water flux and θ predictions under the study site conditions.

The simulation of RZWQM terminates with an error when convergence issues related to the solution of Richards' equation or water balance occur. An incompatible combination of model parameters is considered as one common cause for these issues. With an increasing number of calibrating parameters the risk of non-convergence with a certain combinations of parameters becomes greater. In this study, 3 of the 8 calibration trials for Scenario 1(a) (involving 35 parameters) failed

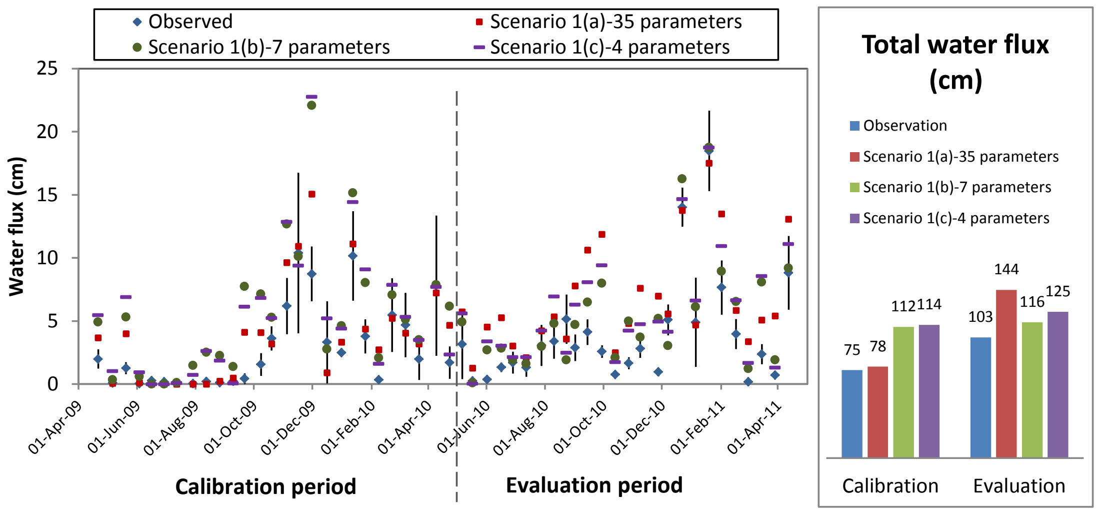

Figure 2.8: Comparison of the averaged observed (±standard deviation of samples in four replicates) and simulated water flux, resulted from calibrating Scenarios 1(a), 1(b) and 1(c) (Case Study 1).

to converge.

The variation of observed water flux was rather high (i.e., the average standard deviation for 53 water flux observations with four replicates for each sampling event was 2.6 cm whereas the mean of all recorded water flux observations was 3.4 cm). Despite this considerable variation, all scenarios reproduced the seasonal trends of water flux relatively well (Figure 2.8). The superior performance of the Scenario 1(a) calibrated model during the calibration period, and the deterioration of its predictions during the evaluation period were also reflected in the cumulative water flux estimation, compared to the two other scenarios. Specifically, for the calibration period (April 2009 to April 2010), Scenarios 1(a), 1(b) and 1(c) estimated the total water flux to be 4, 49 and 52% more than observed values (5 trials for Scenario 1(a), and 8 trials for Scenarios 1(b) and 1(c)). In contrast, the total water flux over the evaluation period was overestimated by 40, 13 and 21% for Scenarios 1(a), 1(b) and 1(c), respectively (Figure 2.8).

The observations from this investigation demonstrate that identification of important parameters through SA is helpful prior to calibration because incorporating an excessive number of parameters increases the risk of over-parameterization. Redundant calibration parameters increase the computational cost of parameterization.

Case Study 2. Field observation and calibration effectiveness

Soil water content (θ) is considered to be a key variable for determining hydrological processes. Measured values of θ are commonly used to calibrate soil hydraulic parameters to improve the prediction of hydrological fluxes such as groundwater recharge, plant water uptake and run off (Vereecken et al., 2008). The availability and quality of θ observations have been improved due to the development of non-destructive measurement techniques, such as remote sensing platforms and soil moisture sensors. In contrast, only a few methods such as those that rely on lysimeters (Grebet and Cuenca, 1991) are available for monitoring water flux below the root zone with minimum impact on natural flow process (Masarik et al., 2004). These methods tend to be challenging and expensive to implement and so are not commonly used for model calibration.

In Case Study 2, results of the current SA were used to design a field experiment with the goal of collecting θ observations from October 2009 to February 2010 (i.e., Fall 2009 and Winter 2010) to calibrate the RZWQM hydraulic parameters. The object of this calibration exercise was to improve water flux estimation at the depth of 60 cm during the period from March to October 2010 (i.e., growing Season 2). The SA results were used to identify the vertical location (soil layer/depth) of θ observation most effective to support this calibration effort. It was expected that calibrating the RZWQM with θ observations that have the most shared sensitive parameters with the water flux process, would improve water flux predictions the greatest. The soil hydraulic parameters influencing water flux the greatest from March to October 2010 were: ρ_b in Soil Layer 1 with 10% total contribution and FC in Soil Layers 1 and 2 with 32 and 3% total contribution, respectively (Figure 2.3). Based on the SA results (Figure 2.5), the average θ in the top 30 cm of the soil profile had the most shared sensitive parameters with the water flux output during the period from March to October 2010 compared with the θ observations at the depths of 45, 60 and 85 cm. Thus the θ data in the upper 30 cm of the soil profile were expected to be the most effective θ observations to calibrate the model for the purpose of water flux predictions at the depth of 60 cm.

To corroborate this decision the RZWQM hydraulic parameters ρ_b, K_{sat} and FC for Soil Layers 1, 2 and 3 were calibrated to θ data under four different scenarios. For each scenario, the set of calibrated parameters were identical, but different sets of θ observations from four soil layers/depths collected from October 2009 to February 2010 (i.e., Fall 2009 and Winter 2010), were employed as historical data. Water flux predictions by the calibrated model for each scenario were then compared with the water flux observations for the period from March to October 2010. No water flux data was utilized in model calibration. The four scenarios were:

- Scenario 2(a). Averaged soil water content data over the upper 30 cm of the soil profile were used. Water content for the depth and time frame was sensitive to ρ_b in Soil Layer 1 and FC in Soil Layers 1, 2 and 3 (Figure 2.5).

- Scenario 2(b). Soil moisture data at the depths of 38 and 56 cm were used. These depths are located in the Soil Layer 2 (25-60 cm), and are close to the SA investigated depths of 45 and 60 cm, respectively. Therefore, θ at these depths is expected to be sensitive to ρ_b for Soil Layer 2 and FC in Soil Layers 2 and 3 (Figure 2.5).

- Scenario 2(c). Soil moisture data at the depth of 75 cm were used. This depth is in the Soil Layer 3 and is close to the SA investigation depth of 85 cm. At this depth and over the applied temporal period, ρ_b in Soil Layer 3 was the only influential parameter on θ (Figure 2.5).

- Scenario 2(d). All soil moisture data including the average θ in the upper 30 cm of the soil profile, and at the depths of 38, 56 and 75 cm were all used.

Five calibration trials (with 250 iterations each) were performed for each scenario. Similar optimization algorithms, calibration criteria (excluding the term for water flux in Eq. 2.16) and parameter ranges as in Case Study 1 were utilized. The calibrated RZWQM from Scenario 2(a) and 2(d) (average RMSE of 2.23, and 2.16, respectively) predicted water flux almost equally well, outperforming Scenarios 2(b) (average RMSE of 2.51) and 2(c) (average RMSE of 2.58) (Figure 2.9). Since the average θ over the upper 30 cm of the soil profile contains information about three important parameters (ρ_b in Soil Layer 1 and FC in Soil Layers 1 and 2), this result is not surprising. In total, these three parameters contribute to 45% of the water flux uncertainty during the evaluation period. This finding conforms to the SA results which show that (1) FC in Soil Layer 2 was the only influential parameter on θ, at the depths of 38 and 56 cm, and as such contributes slightly (3%) to the variation of the water flux during the evaluation period; and (2) θ and water flux at the depth of 85 cm do not share any common influential parameters. The results from this investigation show that under the current study conditions, average θ observations over the upper 30 cm of the soil profile were the most effective θ observation (compared to the θ observations at other depths) to use as historical data when the goal of RZWQM calibration is to predict water flux from March to October 2010. Additional θ observations deeper in the soil profile did not result in improved water flux predictions. Since collecting field data is expensive, time-consuming, and associated with experimental errors, data collection efforts should focus on collecting θ from locations in the soil profile that have the biggest impact on the model output of interest. These relationships can be identified through a SA as shown here.

2.4 Conclusion

In this study, sample-based regression and decomposition methods were used to evaluate the sensitivity of RZWQM key outputs to the uncertainty of input parameters with considering parameters correlations and nonlinear relations. In this

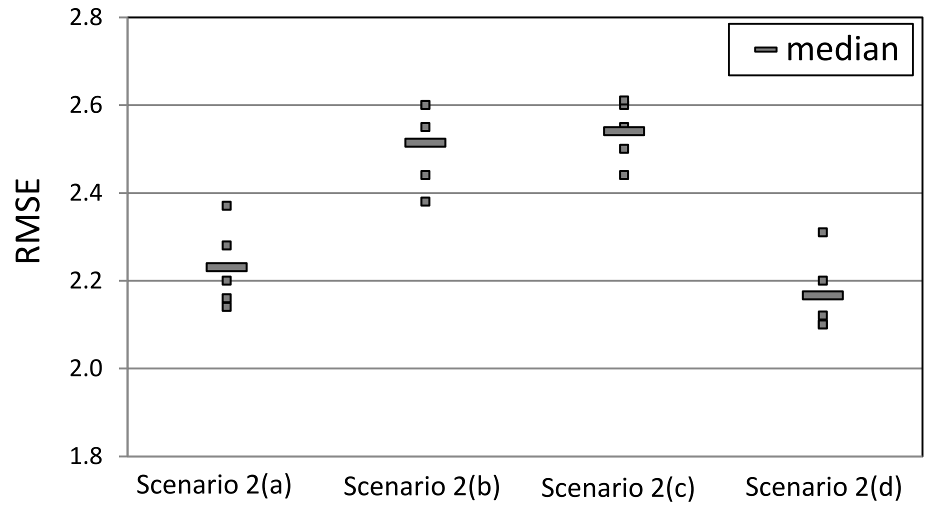

Figure 2.9: Comparison of water flux estimations in the second growing season, obtained from four calibrating scenarios in Case Study 2. In Scenario 2(a), averaged θ over the upper 30 cm of the soil profile were used as the observation data. Observation data in Scenarios 2(b) includes recorded θ at the depth of 38 and 56 cm. Observation data in Scenarios 2(c) includes recorded θ at the depth of 75 cm. All θ observations used in Scenarios 2(a), 2(b) and 2(c) were employed in calibrating Scenario 2(d).

study, not only the parameters' importance was ranked, but also the contribution of individual input parameters to the output uncertainties was apportioned. To the best of authors' knowledge, this is the most comprehensive study to date of SA on the well-known agricultural system model, RZWQM.

The influence of 70 parameters including 35 values of 21 hydrological parameters and 35 nitrogen cycle parameters were tested over various vertical-spatial and temporal domains. Briefly, ρ_b for soil Layer 1, FC for soil Layers 1 and 3 and albedo of the crop were the key parameters affecting water flux and ET. The parameters that had the most influence on the following nitrogen-related outputs: total $NO_3^- - N$ in the soil profile, mineralization, denitrification loss, $NO_3^- - N$ leaching and plant N-uptake were the transient coefficient of fast to intermediate humus pool; C:N ratio of the fast humus pool; OM decay rate of fast humus pool; and FC for Layer 3.

Most of the investigated model parameters had no contribution to the model output uncertainty. This is likely related to the site-specific characterization of soil layers that reduced uncertainty ranges associated with some parameters such as silt and clay fractions for soil Layers 1 and 2. Maximum ranges allowed by the model for the macroporosity parameters (17 parameters) were tested in this SA and the results indicated that selected model outputs were not sensitive to any of these parameters. This is likely due to the sandy soil profile. The correlated contribution of studied parameters to the model output uncertainty was <10%. If these small correlations are neglected, the investigated RZWQM parameters can be considered as independent, and hence their contributions to the uncertainty in the model outputs can be studied independently. The sensitivity of the model outputs to different parameters varied seasonally due to differences in environmental and agricultural factors. For example, crop albedo contributed to 19% of water flux estimation uncertainty in the growing seasons, whereas its contribution in the wet/cold season was negligible. In contrast, the FC for Layer 3 was responsible for 12% of water flux uncertainty in the wet/cold season 1, but it had no influence on water flux uncertainty in the growing seasons. Accordingly, it is recommended to test the sensitivity of model output and calibrate the model under the same conditions.

It was found that calibrating an excessive number of RZWQM hydrological parameters (35 parameters) increased the risk of over-parameterization and deteriorated model predictions. Using SA results, the number of parameters that required calibration was minimized from 35 parameters to as few as four parameters, for which even manual calibration is applicable. This reduces the burden of applying sophisticated automatic calibration methods.

The field observations that have the most shared sensitive parameters with the model output of interest are most effective to use as RZWQM calibration targets. Quantitative SA results can be used to investigate the location and time of such field observations and design appropriate experiments. Under the current study conditions, average θ observations over the upper 30 cm of the soil profile were the most effective θ observation (compared to the θ observations at other depths) to use as the calibration target when the goal of calibration is to improve water flux prediction from March to October 2010.

Chapter 3

Calibration and evaluation of agricultural nitrogen models for simulating soil water flux and nitrate loading below the root zone

Outline

Using modeling tools to simulate the fate and transport of nitrogen in agricultural systems is almost always associated with significant data and calibration requirements. In this study, a step-by-step approach using both automatic and manual calibration methods was developed based on available field data to calibrate selected soil hydraulic, soil organic matter and growth parameters, sequentially. The goal of this study was to compare and study the ability of two agricultural ni-

trogen models, Root Zone Water Quality Model (RZWQM) and CoupModel, to simulate water flux and nitrate loading below the root zone. The field data used for this modeling investigation were collected from an experimental raspberry field, located over the Abbotsford-Sumas Aquifer where elevated groundwater nitrate concentration is attributed to nutrient application practices that are associated with raspberry production. Calibrated RZWQM and CoupModel both simulated water flux well; however, calibrated RZWQM (RMSE 1.98 cm) rather outperformed the CoupModel (RMSE 2.53 cm). It was found that the superior performance of the calibrated RZWQM is related to both application of a better evapotranspiration model and utilization of a more effective calibration algorithm compared to the CoupModel. Calibrated CoupModel using the logistic and the water use efficiency approaches simulated nitrate loading time series better than RZWQM, on average, by 34%. Overall, it was found that information regarding soil organic matter and growth parameters is vital for reliable application of models. With such information, the CoupModel and the RZWQM (to lesser extent) were found to be reliable tools to simulate nitrate loading below the raspberry root zone.

3.1 Introduction

Agricultural nitrogen models are potentially useful to understand nitrogen processes, and to develop strategies that aim at mitigating nitrate loading to groundwater. The availability and use of these models for nitrogen management has increased rapidly (Shaffer et al., 2001; Šimnek, 2005). Agricultural nitrogen models represent an array of physical, chemical and biological processes and thus tend to be complex and contain many parameters (Ahuja and Ma, 2002). Soil hydraulic parameters are among essential requirements of most agricultural models (e.g., LEACHM (Hutson and Wagenet, 1992), DAISY (Abrahamsen and Hansen, 2000), WAVE (Vanclooster et al., 1994) and NTRM (Shaffer and Pierce, 1987)). These parameters control soil moisture content which influences microbial activities (Linn and Doran, 1984) and nitrogen transformations in the root zone. More importantly, they control soil moisture dynamics which directly governs nitrate transport either towards the plant (N-uptake) or away from the plant (loss). Soil hydraulic parameters are highly variable and depend on soil characteristics. In some models, default values for soil hydraulic parameters can be obtained from an available database or estimated from pedo-transfer functions. These parameters, however, refer to the most common soils, and only facilitate general application of the models. A more sophisticated method for defining soil hydraulic parameters is calibration. Most calibration studies employ traditional trial-and-error methods; however, calibration of models with many parameters is time-consuming and subjective. To tackle this problem, automatic calibration methods have been proposed as repeatable and objective ways to estimate parameters (Madsen et al., 2002; Vrugt et al., 2008). The common cost of model calibration includes thousands of model evaluations and having enough field observations which are likely only affordable in research-level studies. Therefore, when using models, it is always of question whether readily available and easily accessible default hydraulic parameters can provide credible simulation results, and if calibration is worth the cost of time and effort.

Discrepancies between simulated and measured soil mineral nitrogen are mainly related to mineralization of soil organic matter (SOM) and plant N-uptake (Johnsson et al., 1987). Therefore, estimating the parameters that govern these crucial nitrogen source/sink terms is an important part of model application. Parameters that control nitrogen cycle and production of nitrate may include SOM pool sizes and rate coefficients associated with various processes. SOM pool sizes are site-specific and difficult to measure. Usually, calibration of these parameters is required (Shaffer et al., 2001). Rate coefficients can be derived from literature values or calibrated from available data sets (Shaffer et al., 2000). Quantification of plant N-uptake has remained a challenge after decades of field trials (Ma et al., 2008). In agricultural models, N-uptake is generally determined based on N-demand and N-supply. Plant N-demand, known as potential N-uptake is specific to the crop and site, and calibration is usually needed to infer the value of this parameter (Ma et al., 2008).

The shallow unconfined Abbotsford-Sumas Aquifer straddles the lower Fraser Valley in southwestern British Columbia, Canada and the Nooksack lowlands in northern Washington State, USA, and provides water for nearly 100,000 people in Canada and 10,000 people in the United States (Mitchell et al., 2003). The fertile well-drained soil has made the area an intensive agricultural region, with raspberries being the predominant crop above the Canadian portion of the aquifer (Hii et al., 1999). Nutrients application practices, associated with raspberry production, have been identified as a major source of nitrate contamination of the aquifer (Mitchell et al., 2003; Zebarth et al., 1998; Wassenaar, 1995). Although, many studies have been performed to understand the nitrogen sources, and to quantify its transformation and transport to the Abbotsford-Sumas Aquifer (Wassenaar et al., 2006; Zebarth et al., 2002, 1999, 1998; Wassenaar, 1995; Zebarth et al., 1995), the role of agricultural models in these investigations has been minimal.

The main objective of this study was to evaluate the ability of two agricultural nitrogen models: Root Zone Water Quality Model (RZWQM) (Ahuja et al., 2000a) and CoupModel (Jansson and Karlberg, 2012) to simulate water flux and nitrate loading from the raspberry root zone. Both models are detailed research models (Shaffer, 2002) that feature complex soil hydrological and nitrogen cycle processes for cropped systems.

Required field data for this study were obtained from an experimental raspberry farm with three different irrigation and nitrogen application combination practices over a two-year study period starting April 2009 and ending April 2011 (Kuchta, 2012). In this modeling study, selected soil hydraulic, SOM and growth parameters were calibrated sequentially. Through this step-by-step calibration process, annual nitrogen mineralization and raspberry N-uptake were also identified for each treatment. According to previous studies (Kowalenko and Hall, 1987; Kowalenko, 1989; Zebarth et al., 1995), nitrogen mineralization on agricultural fields in the Lower Fraser Valley is highly variable. Dean et al. (2000) estimated mineralization at 43 kg ha^{-1} during early spring on a raspberry field and concluded that mineralization can supply plant N-uptake or contribute to nitrate loading. Some studies have been carried out to understand and quantify raspberry N-uptake under different nitrogen application rates and timing (Dean, 1987; Rempel et al., 2004). N-uptake pattern by the above-ground tissues of the raspberry crop in the Lower Fraser Valley was found to be inconsistent, ranging from 85 to 122 kg ha^{-1} annually (Kowalenko, 1994).

Initially selected soil hydraulic parameters were calibrated. Due to large number of soil hydraulic parameters that were calibrated in this study, automatic calibration methods were used. The RZWQM and the CoupModel have been used in various calibration and evaluation studies. Only in a few studies has automatic parameter estimation methods been used with the RZWQM (Fang et al., 2010; Nolan et al., 2010; Malone et al., 2010). Two automatic calibration methods including Generalized Likelihood Uncertainty Estimation (GLUE) and Bayesian calibration methods are provided in the CoupModel, and have been used in related studies (Svensson et al., 2008; Conrad and Fohrer, 2009; Nylinder, 2010). The predictive ability of the RZWQM and the CoupModel to simulate water flow was compared using calibrated and default soil hydraulic parameters. Following calibration of the soil hydraulic parameters and maximizing the ability of both models for simulating water flow, the SOM and growth parameters were calibrated. For these parameters, a manual trial-and-error method was adopted, using statistical and graphical criteria to evaluate model performance. Finally, the predictive ability of the models to simulate the nitrate loading time series over the two-year study period was investigated using all calibrated parameters.

3.2 Materials and Methods

3.2.1 Site Description

The experimental data set was provided by Kuchta (2012). The goal of this study was to understand the linkages between raspberry production and nitrate loading

Table 3.1: Soil horizon information based on the field survey and laboratory characterization.

Depth (cm)	Layer	Description	Gravel (%)	Sand (%)	Silt & Clay (%)
0-25	1	Loam	4	26	70 (with 6 to 11 clay)
25-60	2	Loam	5	31	64 (with 3 to 5 clay)
60-100	3	Sand	30	70	0

to groundwater in the Abbotsford-Sumas Aquifer. Raspberries have unique growth and fruiting characteristics. The plant's canes are biennial, while its roots and crown are perennial. Each spring, new above-ground canes called primocanes develop. These canes grow vegetatively during the first season, and produce fruit during the summer of the next year. The previous season's canes called floricanes die shortly after fruiting (Crandall, 1995). A brief description of the experimental field and relevant measurements are described below.

3.2.2 Field Data

The experimental raspberry farm was established at the Clearbrook sub-station, Agriculture and Agri-Food Canada (AAFC), in Abbotsford, BC, Canada in 2008. The surficial soil layer at the study site is tenuous and well-drained due to its sandy texture, and is underlain by the shallow unconfined glacial-fluvial Abbotsford Aquifer. Detailed soil horizon information including the thickness of the different soil layers and texture classification of the upper 1 m is given in Table 3.1. The average annual precipitation is 1570 mm, and the average monthly temperature ranges from 2.6 °C in January to 17.7 °C in August with an annual average of 10.0 °C. The annual precipitation in the study period from April 2009 to April 2010 (Y1) and April 2010 to April 2011 (Y2) was 1417 and 1613 mm, respectively (Environment Canada, 2012b).

The experiment compared different agricultural management systems (nitrogen application, irrigation and inter-row cultivation management) using completely randomized design with four replicates. In this study, we applied the RZWQM and the CoupModel to the data collected from three treatments identified as CON-0 (conventional drip irrigation with no nitrogen fertilizer), CON-100 (conventional drip irrigation with nitrogen fertilizer applied at the rate of 100 kg N ha^{-1}) and SCH-100 (scheduled drip irrigation with nitrogen fertilizer applied at the rate of 100 kg N ha^{-1}). Treatment SCH-100 was irrigated in accordance with the estimated evapotranspiration (ET) using an automated atmometer (Colorado State University Cooperative Extension, 1999) and soil moisture content, whereas the conventional irrigation for treatments CON-0 and CON-100 was based on the common or local growers' practice for raspberry production. The total amount of irrigation in the conventional and scheduled irrigated treatments was 714 and 381 mm in Y1, and 796 and 391 mm in Y2, respectively. Raspberries in treatment CON-100 and SCH-100 received 100 kg N ha^{-1} as urea in April and May of 2009 and 2010. The agriculture practice for treatment CON-100 mimics the growers' common practice across the region. Raspberries are usually planted in rows, and at this study site the rows were spaced 3 m apart. The inter-rows of all plots were clean-cultivated. Before each growing season, pruned raspberry canes were ploughed into the soil on the raspberry inter-rows. The background SOM was measured before plot establishment in 2008 as 0.0325 gr OM gr^{-1}soil. A network of passive capillary wick samplers (PCAPS) (Jabro et al., 2008) was installed in and between raspberry rows at a depth of 55 cm (top of the gravelly sand aquifer) as shown in Figure 3.1. The PCAPS were designed to collect the drainage soil water over an area of 60 $\times$ 60 cm. The volume and nitrate content of the captured water were measured bi-weekly for a total of 53 observational points.

The soil moisture capacity associated with 5 pressure points, ranging from 10 to 40 kPa, were determined for each soil layer using a pressure plate (ASTM C1699-09, 2009; Richards, 1965, 1948). For this investigation, two intact soil samples were collected for each soil layer from two different locations within the study site. The Brooks and Corey (1964) parameters including pore size distribution index (λ), air-entry water suction (ψ_b), saturation water content (θ_s), residual water content (θ_r),

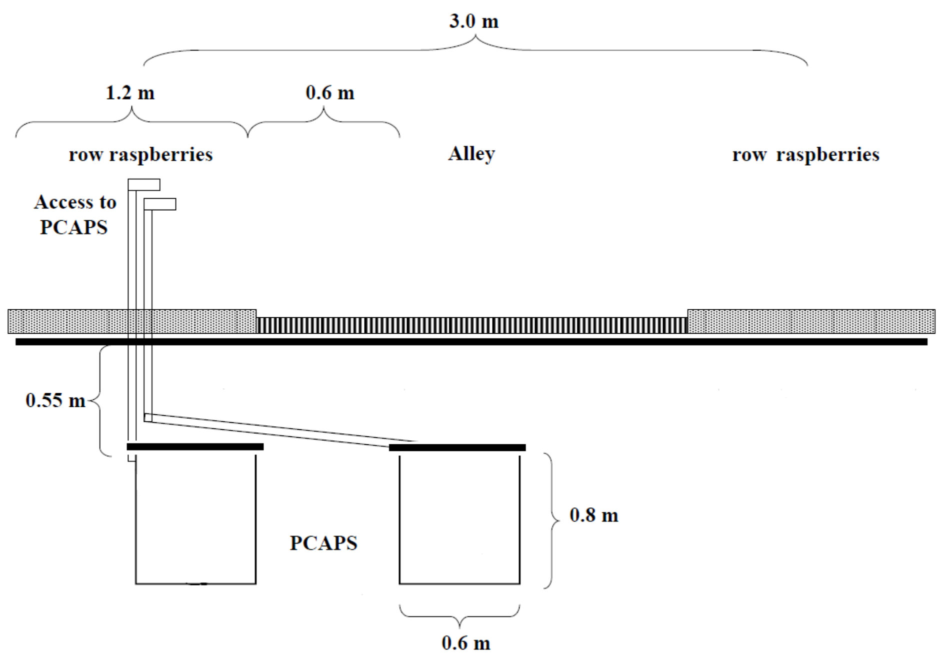

Figure 3.1: PCAPS installation under raspberry row and inter-row (adopted from Kuchta (2012)).

and moisture content at -33 kPa, known as field capacity (FC) (Nachabe, 1998) were defined by fitting a curve, known as soil moisture retention curve (SMRC) to these data points (Table 3.2). Soil bulk density for each soil layer was determined from dry weight and the volume of each soil sample. Saturated hydraulic conductivity (K_{sat}) of each soil layer was measured using the Guelph Permeameter (Reynolds and Elrick, 1985).

3.2.3 Model Description

The RZWQM and the CoupModel are designed for the assessment of nitrogen management practices on crop growth, and soil water and nitrogen balances; however, the complexity and treatment of individual processes are different. The structure and features of both models have been reviewed in numerous studies (Moriasi et al., 2012; Heinen, 2003; Šimnek, 2005). Köhne et al. (2009) studied the weakness and

Table 3.2: Selected parameters used in the automatic calibration of the CoupModel and RZWQM. The default parameter values for the CoupModel were defined from the pedo-transfer function as proposed by Rawls and Brakensiek (1989), and the default parameter values for the RZWQM were adopted from the model database based on soil texture (Rawls et al., 1982). Calibration bounds were determined from recommended/literatures values (Ahuja et al., 1988; Rawls et al., 1982) and were adjusted due to the existence of significant amount of humus in the upper soil layer and gravel in the entire soil profile. Saturated hydraulic conductivity was measured using Guelph Permeameter.

Parameter	Soil layer	Unit	Measured	Default	Calibration range
		RZWQM			
Soil bulk density - ρ_b	1	g cm^{-3}	1.0	1.322	1.0 - 1.42
	2		1.13	1.322	1.13 - 1.42
	3		2.1	1.492	1.49 - 2.0
Saturated hydraulic conductivity - K_{sat}	1	cm hr^{-1}	1.81	0.68	1.32 - 8.33
	2		2.48	0.68	1.32 - 8.33
	3		70.5	21.0	21.0 - 81.36
Soil moisture content at -33 kPa - FC	1	cm^{3}cm^{-3}	0.1	0.28	0.2 - 0.3
	2		0.2	0.28	0.2 - 0.3
	3		0.06	0.06	0.02 - 0.1
		CoupModel			
Pore size distribution index - λ	1	-	0.85	0.36	0.01 - 0.58
	2		0.48	0.38	0.01 - 0.58
	3		0.9	0.53	0.01 - 1.31
Air-entry water suction - ψ_b	1	cm	38	30	0.01 - 160.5
	2		45	26	0.01 - 160.5
	3		20	7	0.01 - 47.4
Saturation water content - θ_s	1	cm^{3}cm^{-3}	0.45	0.5	0.28 - 0.64
	2		0.42	0.5	0.28 - 0.64
	3		0.3	0.44	0.31 - 0.56
Residual water content - θ_r	1	cm^{3}cm^{-3}	0.01	0.04	0.001 - 0.121
	2		0.01	0.03	0.001 - 0.058
	3		0.04	0.03	0.001 - 0.058
Saturated hydraulic conductivity - K_{sat}	1	cm hr^{-1}	1.81	0.9	1.32 - 8.33
	2		2.48	1.3	1.32 - 8.33
	3		70.5	34	21.0 - 81.36

strengths of these models for the simulation of preferential flow and non-equilibrium non-reactive solute transport. According to Köhne et al. (2009), the RZWQM uses the "gravity preferential model" which assumes that flow in the preferential domain is controlled only by gravity and is always directed downward. This flow model, however, only fits to the soils with heavy clay soils with notable cracks (Köhne et al., 2009). The CoupModel, on the other hand, uses the empirical capacity approach for preferential flow which assumes that downward flow from each soil layer is zero until it is filled to its moisture capacity. This model is applicable for specific conditions only. Wu and Kersebaum (2008) reviewed simulation models including the RZWQM and CoupModel to demonstrate the advantages and disadvantages of the approaches they use to calculate different processes. According to Wu and Kersebaum (2008), it is useful to include the contribution of organic nitrogen to plant nitrogen supply under cold climate conditions or when mineral nitrogen input is low. The RZWQM does not consider organic nitrogen as a source of plant nitrogen supply; however, this process was recently incorporated in the CoupModel. The performance of the two agricultural models to simulate soil water and nitrogen dynamics, however, has not been compared with the same data set. The main components of these two models are discussed below.

3.2.3.1 RZWQM

The one-dimensional RZWQM is an integrated physical, chemical and biological process model that simulates water and solute movement, heat flux, plant growth and nitrogen and carbon turnover as the result of soil management activities (Ahuja et al., 2000a). In the RZWQM, soil hydraulic parameters are described with the Brooks and Corey (1964) relationships while water distribution is calculated using Richards' equation. The model can account for macropore flow with a concept similar to the transient flow models of Hoogmoed and Bouma (1980), and Beven and Germann (1981). The extended Shuttleworth-Wallace model is used to simulate ET (Farahani and Ahuja, 1996). Root water uptake is simulated using the approach of Nimah and Hanks (1973). SOM is partitioned into five computational pools based on their physical and chemical properties: fast and slow residue pools; and fast, intermediate and slow humus pools. Material in an organic matter pool can be transformed into other pools, assimilated into microbial biomass or emitted as CO_2. Decomposition of SOM is modeled as a first-order reaction. RZWQM is implemented with a Generic Crop Growth Model and DSSAT 4.0 Crop growth model (Tsuji et al., 1994). However, when woody perennial agriculture crops are simulated, RZWQM only mimics plant growth by taking water and nutrients from the soil using a simple module, Qckplant, which does not simulate photosynthesis and yield, and only simulates the environmental impacts of the cropping system. It requires definition of a limited number of parameters including length of the growing season, leaf area index, winter dormancy recovery date, seasonal potential N-uptake (i.e., N-demand) and litter fall. Seasonal N-demand is partitioned into daily values. Therefore, plant N-uptake is relative to N-demand and soil N-availability. A comprehensive description of this model is provided by Ahuja et al. (2000c).

3.2.3.2 CoupModel

The one-dimensinal CoupModel or Coupled Model (Jansson and Karlberg, 2012), formerly known as SOIL or SOILN-models (Eckersten et al., 1998), simulates coupled fluxes of heat and water in a layered soil profile. In the CoupModel, nitrogen and carbon turnover, and plant development are also simulated. The soil water retention function is expressed with either the Brooks and Corey (1964) or van Genuchten (1980) function, and the soil water movement is simulated using Richards' equation. Soil macropores are accounted in the model with an implicit relationship that partitions infiltration into ordinary Darcy flow and bypass flow. Snow, intercepted water, and surface ponding occur at the upper soil boundary. Nitrogen enters into the soil system from above (as plant litter, dry/wet deposition and fertilizer) and below the ground surface (SOM decomposition). SOM is partitioned into a humus pool, litter pool, surface litter pool and faeces pool (if manure is applied). When litter falls, it first enters the microbial-inactive surface litter pool, and then gradually enters the litter and humus pools. In the CoupModel there are different approaches to calculate plant growth or biomass production (leaf assimilation). Assimilated carbon allocates to different parts of the plant: root, leaf, stem and grain. The carbon content in different parts of the plant gives rise to N-uptake and allocation in accordance with the parameterized C:N ratio. Inorganic-N dynamics are simulated based on the nitrogen cycle, soil mineral nitrogen content, and soil water flow in different soil layers. A detailed description of this model is given by Jansson and Karlberg (2012).

3.2.4 Model Application and Parameterization

3.2.4.1 General approach

The general stages that were taken to calibrate and evaluate the two models are shown in Figure 3.2. The first stage comprised the calibration of the selected hydraulic parameters (including 9 and 15 parameters for RZWQM and CoupModel, respectively (Table 3.2)) for Y1. In the second stage, which involved the calibration of selected SOM parameters, data from the inter-rows (without the effect of fertilizer or crop) were utilized. This stage is consistent with Duwig et al. (2003); Houot et al. (1989), and Knisel and Turtola (2000) who used data collected on bare soil plots to identify SOM parameters and the mineralization rate. Finally, growth parameters were adjusted and seasonal plant N-uptake was modified for each treatment. The calibration parameters for the RZWQM were selected based on the outcomes of a sensitivity analysis (see Chapter 2) that was performed to identify the most influential parameters in the RZWQM for key model outputs. For the CoupModel, calibration parameters were selected based on the results of a previous sensitivity analysis conducted by Conrad and Fohrer (2009). Detailed assumptions and settings for the application of CoupModel and RZWQM are described below.

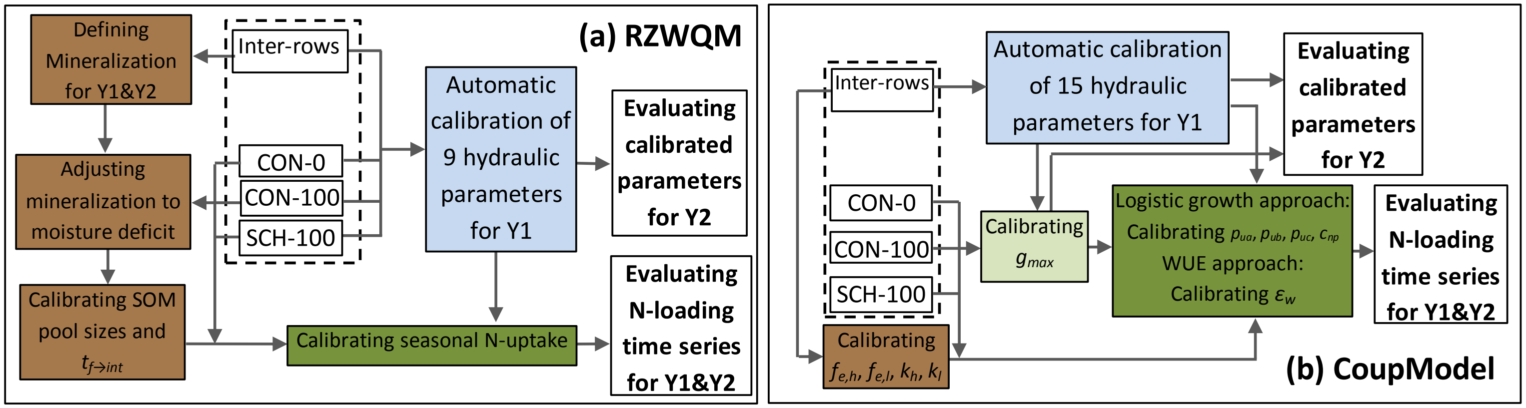

Figure 3.2: Calibration and evaluation stages for (a) RZWQM, and (b) CoupModel. The dashed box represents the field data that were used for parameter calibration. For the RZWQM, selected hydraulic parameters were calibrated using row and inter-row data in Y1, and evaluated for simulating water flux in Y2. Mineralization rate was defined from the inter-rows data and then adjusted based on soil moisture difference between row and inter-row during the growing seasons of Y1 and Y2. In the next step, SOM pool sizes and $t_{f\rightarrow int}$ were calibrated using data from all three treatments. In the final stage, seasonal plant N-uptake for each treatment was modified for Y1 and Y2 separately, and the performance of the model to simulate nitrate loading time series using all calibrated parameters was evaluated. For the CoupModel, 15 hydraulic parameters were calibrated using inter-rows data in Y1. Then g_{max} was simultaneously modified for the three treatments. Calibrated hydraulic parameters and g_{max} were evaluated for simulating water flux in Y2. Using inter-rows data from Y1 and Y2, selected SOM parameters including $f_{e,h}$, $f_{e,l}$, k_h, k_l were calibrated. In the final step, plant growth parameters related to the logistic growth approach (i.e., p_{ua}, p_{ub}, p_{uc}, cn_p) and the WUE approach (i.e., ε_w) were modified simultaneously for the three treatments. The performance of the model for predicting nitrate loading fluctuations using all calibrated parameters was evaluated.

3.2.4.1.1 RZWQM Daily maximum and minimum air temperature, wind speed, relative humidity and precipitation data were obtained from the Abbotsford Airport weather station. The RZWQM climate generator was used to randomly generate shortwave radiation data for the nearest weather station (i.e., Concrete, WA, USA). A modified version of Brooks-Corey relationship (Williams and Ahuja, 1992), known as one-parameter method, was used to describe soil moisture retention properties and unsaturated hydraulic conductivity. This method requires soil moisture content at -33 kPa, FC (Nachabe, 1998). A unit hydraulic gradient was assumed as the lower boundary condition. Nine soil hydraulic parameters (Table 3.2) were calibrated on both raspberry rows and inter-rows during Y1 using the Dynamically Dimensioned Search (DDS) optimization algorithm (Tolson and Shoemaker, 2007) with 5 trials and 250 model evaluations for each calibration trial. The root mean square error (RMSE) was used as the model calibration criteria to evaluate the simulation results. Parameter bounds were determined from recommended/literature values (Ahuja et al., 1988; Rawls et al., 1982) in accordance with the soil data (Table 3.1). Since there is a significant amount of humus in the upper soil layers, the soil bulk density (ρ_b) ranges were justified. Also, due to existence of a rather significant amount of gravel in the soil, the saturated hydraulic conductivity (K_{sat}) values were adjusted (Smith and Mullins, 2001; Clapp and Hornberger, 1978). The default values for the hydraulic parameters were adopted from the RZWQM database based on soil texture class of each layer (Rawls et al., 1982). Calibrated hydraulic parameters were used to predict the water flux in Y2, and these results were evaluated against the PCAPS data.

Due to clean-cultivation, the major nitrogen sinks and sources for the raspberry inter-rows included leaching, mineralization and atmospheric deposition. Preliminary model simulation results indicated that denitrification is negligible. Average atmospheric deposition in the Abbotsford region of 8.6 kg ha^{-1} per year (Environment Canada, 1997) was deducted from the inter-rows PCAPS nitrate loading data. The result was adopted as net mineralization for the raspberry inter-rows. SOM background, litter fall and climate conditions were comparable between raspberry rows and inter-rows; therefore, the estimated mineralization from the inter-rows was adopted as the mineralization for the raspberry rows. However, due to lack of irrigation and soil moisture on the inter-rows, mineralization would expected to be underestimated for the irrigating seasons on the raspberry rows. To address this problem, the estimated mineralization from the inter-rows was adjusted according to the soil moisture deficit between the rows and inter-rows during irrigating seasons of Y1 and Y2 using (Myers et al., 1982):

$$\frac{Y}{Y_{max}} = \frac{W - W_0}{W_{max} - W_0} \tag{3.1}$$

where Y is the estimated mineralized nitrogen from the inter-rows during the irrigating season, W is the average soil moisture content on raspberry inter-rows during the irrigating season, Y_{max} is the adjusted mineralized nitrogen on raspberry rows, W_{max} is the average soil moisture content on raspberry rows during the irrigating season and W_0 is the soil moisture content at -4.0 MPa. W and W_{max} were estimated by the RZWQM using the calibrated hydraulic parameters.

Four soil organic parameters: the transition coefficient of the fast to intermediate humus pool ($t_{f \rightarrow int}$) and the fast, intermediate and slow SOM pool sizes were modified to reproduce the adjusted mineralization rates on the raspberry rows for each treatment for Y1 and Y2. It was assumed that 100 kg ha^{-1} per year (selected based on the RZWQM database for raspberries) of plant residue is incorporated into the soil after each growing season. Finally, the calibrated soil hydraulic and SOM parameters were used, and the effect of raspberry production on nitrate load from the root zone was simulated using Qcktree. The start and end dates of the growing season were set to Day 90 and 270, respectively. The maximum leaf area index (LAI) was set to 4 (Scurlock et al., 2001). The potential plant N-uptake in Y1 and Y2 growing seasons was manually calibrated, separately for each treatment, using the PCAPS nitrate data. The step-by-step calibration and evaluation procedure for the RZWQM is shown in Figure 3.2a.

3.2.4.1.2 CoupModel Meteorological data including daily precipitation, wind speed, average temperature and relative humidity data were extracted from the Abbotsford Airport weather station data. Average cloudiness parameter (65%) was taken from Natural Resources Canada (2012), and used in the model to estimate radiation. The Brooks and Corey (1964) function was selected to express the water retention function and the unsaturated hydraulic conductivity. A unit gradient was assumed as the lower boundary condition. Fifteen soil hydraulic parameters (Table 3.2) were calibrated on the raspberry inter-rows during Y1 using the Generalized Likelihood Uncertainty Estimation (GLUE) approach (Beven and Binley, 1992) with 5000 trials. The RMSE was used as the CoupModel efficiency measure. The lowest 10% RMSE was accepted as the behavioral parameter combinations. The RMSE measures of the accepted runs were rescaled to determine their cumulative distribution function (CDF). The median and the 90% confidence bound (i.e., values within the 5th and 95th percentiles of all accepted runs) of the CDF distribution were accepted as the deterministic model prediction and the associated uncertainty, respectively (Blasone et al., 2008). Available knowledge on each soil layer was used to set the parameter bounds based on Ahuja et al. (1988) and Rawls et al. (1982). Similar to RZWQM, a significant amount of humus in the upper soil layers and gravel in the entire soil profile were accounted for in the parameters bounds set for ρ_b and K_{sat}. The default values of the calibrated parameters were estimated for each soil layer by using the pedo-transfer function proposed by Rawls and Brakensiek (1989) (Table 3.2). Calibrated parameters were evaluated for Y2 by simulating soil water flux on raspberry inter-rows.

After calibration of the selected hydraulic parameters on the inter-rows, SOM parameters including the decay efficiency of litter ($f_{e,l}$) and soil humus ($f_{e,h}$) pools, and the rate coefficient of litter (k_l) and soil humus (k_h) pools were manually adjusted using PCAPS nitrate data for Y1 and Y2 on the inter-rows. Atmospheric nitrogen deposition (Environment Canada, 1997) was introduced to the model with two parameters: dry deposition of mineral N (0.001 g N m^{-1}day^{-1}) and concentration of mineral N in precipitation (0.34 mg N L^{-1}). Microbes were represented implicitly; that is, decomposition of organic matter (litter and humus pools) was substrate controlled, and follows a first-order rate governed by the response functions of soil temperature and moisture. A common soil temperature response function (Ratkowsky et al., 1982) and a standard soil moisture response function (Jansson and Karlberg, 2012) were used. To account for litter fall on the inter-rows, an amount of 2.1 and 4.2 g N m^{-2} per year with an average C:N ratio of 35 was introduced to the CoupModel as plant N-litter in fall of Y1 and Y2, respectively. These N-litter rates were determined from preliminary model simulations of the raspberry rows, where, the estimated plant N-litter from the raspberry row was partitioned between rows and inter-rows areas in accordance with the row-spacing. The validity of the adopted N-litter fall was examined against final modeling results using all calibrated parameters.

The calibrated soil hydraulic and organic matter parameters were used to simulate growth on the raspberry rows. The Penman-Monteith equation (Monteith, 1965) was used to simulate ET on the rows. The canopy resistance in the Penman-Monteith equation is proportional to the maximum leaf conductance of fully open stomata (g_{max}) and leaf area index (A_l). Leaf area index (A_l) was set to 4 (Scurlock et al., 2001). The start and end dates of plant N-uptake were set to Day 90 and 270. Observed PCAPS water data from the raspberry rows were used to calibrate g_{max}, and a single value was estimated for all treatments for Y1. The calibrated hydraulic parameters and gmax were evaluated by comparing estimated water flux with PCAPS data for Y2 on the raspberry rows. To simulate plant carbon assimilation, two different approaches were used:

1. The logistic growth approach (Johnsson et al., 1987) in which carbon assimilation is proportional to the potential N-uptake as given by:

$$C_{Atm \to a} = cn_p . f\left(\frac{T_a}{T_p}\right) . N_{pl,p} . t \tag{3.2}$$

with

$$N_{pl,p} = \frac{p_{ua}.p_{uc}.\frac{p_{ua}-p_{ub}}{p_{ub}}.e^{-p_{uc}.\Delta t}}{\left(1 + \frac{p_{ua}-p_{ub}}{p_{ub}}.e^{-p_{uc}.\Delta t}\right)^2} \tag{3.3}$$

where cn_p is the C:N ratio of the assimilated biomass; $f\left(\frac{T_a}{T_p}\right)$ is the response function for soil water stress; T_a is actual transpiration; T_p is potential transpiration; p_{ua} is the potential N-uptake (g m^{-2}); p_{ub} and p_{uc} are shape factors; and Δt is the time since the start of growth. Potential N-uptake (p_{ua}), p_{ub}, p_{uc} and cn_p were calibrated manually against the PCAPS nitrate data observations. For each of p_{ub}, p_{uc} and cn_p parameters, a single value was identified for all three treatments, whereas p_{ua} was calibrated separately for each treatment and for each growing season.

2. The water use efficiency (WUE) approach (Karlberg et al., 2006) in which the actual transpiration is the driving force of the carbon assimilation by plants as given by:

$$C_{Atm \to a} = \varepsilon_w.\eta.T_a \tag{3.4}$$

where ε_w is the WUE coefficient, and η is the conversion factor for biomass to carbon. WUE coefficient (ε_w) was calibrated manually using PCAPS nitrate data for Y1 and Y2 growing seasons for each treatment.

The calibration and evaluation procedure for the CoupModel is shown in Figure 3.2b.

3.2.4.2 DDS vs. GLUE

Since two different algorithms were used for the calibration of the RZWQM and the CoupModel, the performance the two calibration methods were compared under equal conditions (that is, by applying the algorithms to a single model) in order to investigate whether significantly different outcomes are generated. Unfortunately, the Coupmodel is available only in GUI environment and application of DDS requires access to model ascii files. Hence, the performance of the GLUE and DDS optimization algorithms to calibrate nine hydraulic parameters in the RZWQM (Table 3.2) was investigated. PCAPS water flux data for Y1 and Y2 collected from treatment CON-100 were used as the target observational data. The number of model evaluations for optimization was set at 5000. Similar parameter bounds as defined in 3.2.4.1.1 were used. Also, the deterministic model prediction for the CoupModel was determined as described in 3.2.4.1.2.

3.2.4.3 Brooks Corey relationship: one-parameter method vs. full-parameter method

Since the one-parameter method of the Brooks-Corey relationship is simple and less parameter-demanding, it was used to obtain soil moisture characteristic curves in the RZWQM. Whereas, the CoupModel used the full-parameter method since it was the only available option for the Brooks-Corey relationship in this model. According to Fang et al. (2010) the one-parameter method (used in the RZWQM) predicts soil moisture content as good as the full Brooks-Corey parameter method (used in the CoupModel) under fallow conditions. Also, Ma et al. (2009) concluded that soil water balance simulation with the RZWQM does not depend on the Brooks-Corey method. Nevertheless, to investigate whether using different representations of the Brooks-Corey relationship can influence the RZWQM water flux estimation and as a result bias the comparison of the performance of the two models for the simulation of water flux, the full-parameter Brooks-Corey method was utilized to simulate water flux for the inter-rows and rows of the three treatments for Y1 and Y2. Results were compared to those generated using the one-parameter method.

3.3 Results and Discussion

3.3.1 Calibration of Hydraulic Parameters and Water Flux Estimation

Selected soil hydraulic parameters in the RZWQM (Table 3.2) were calibrated on the raspberry rows and inter-rows for treatments CON-0, CON-100 and SCH-100, separately in Y1. PCAPS water flux data were used as the calibration targets. Out of the five DDS trials, the calibrated model with the best water flux estimation (with the lowest RMSE) was selected for the inter-row and rows for each treatment. These calibrated hydraulic parameters were then utilized to simulate water flux on raspberry rows and inter-rows in Y2, and results were compared to the PCAPS water flux observations (Figure 3.3). The general trends in water flux were reproduced rather well by the RZWQM with an average RMSE of 1.98 cm for all the investigated treatments on raspberry rows and inter-rows during Y2 (Figure 3.3). Compared to the simulations obtained by using the default parameter set, the RMSE improved using the calibrated hydraulic parameter set for Y1 (i.e., 32, 33, 36, and 24% on the inter-rows and rows in treatments CON-0, CON-100 and SCH-100, respectively) and Y2 (i.e., 41, 9, 18, and 18% on the inter-rows and rows in treatments CON-0, CON-100 and SCH-100, respectively) (Figure 3.3). This suggests that calibration was effective; that is, calibration improved water flux estimation compared to the results that were obtained from the RZWQM available hydraulic parameters.

Since all the inter-rows for treatment CON-0, CON-100 and SCH-100 were treated the same, no difference was expected in the collected PCAPS data. Selected soil hydraulic parameters in the CoupModel (Table 3.2) were calibrated using the average inter-rows PCAPS water flux data for Y1. Out of 5000 CoupModel runs, 638 runs were accepted as behavioral parameter combinations (retained in the lowest 10% RMSE). The 90% confidence bound of the accepted runs (i.e., simulated values within the 5^{th} and 95^{th} percentiles of all accepted runs) was small with min-

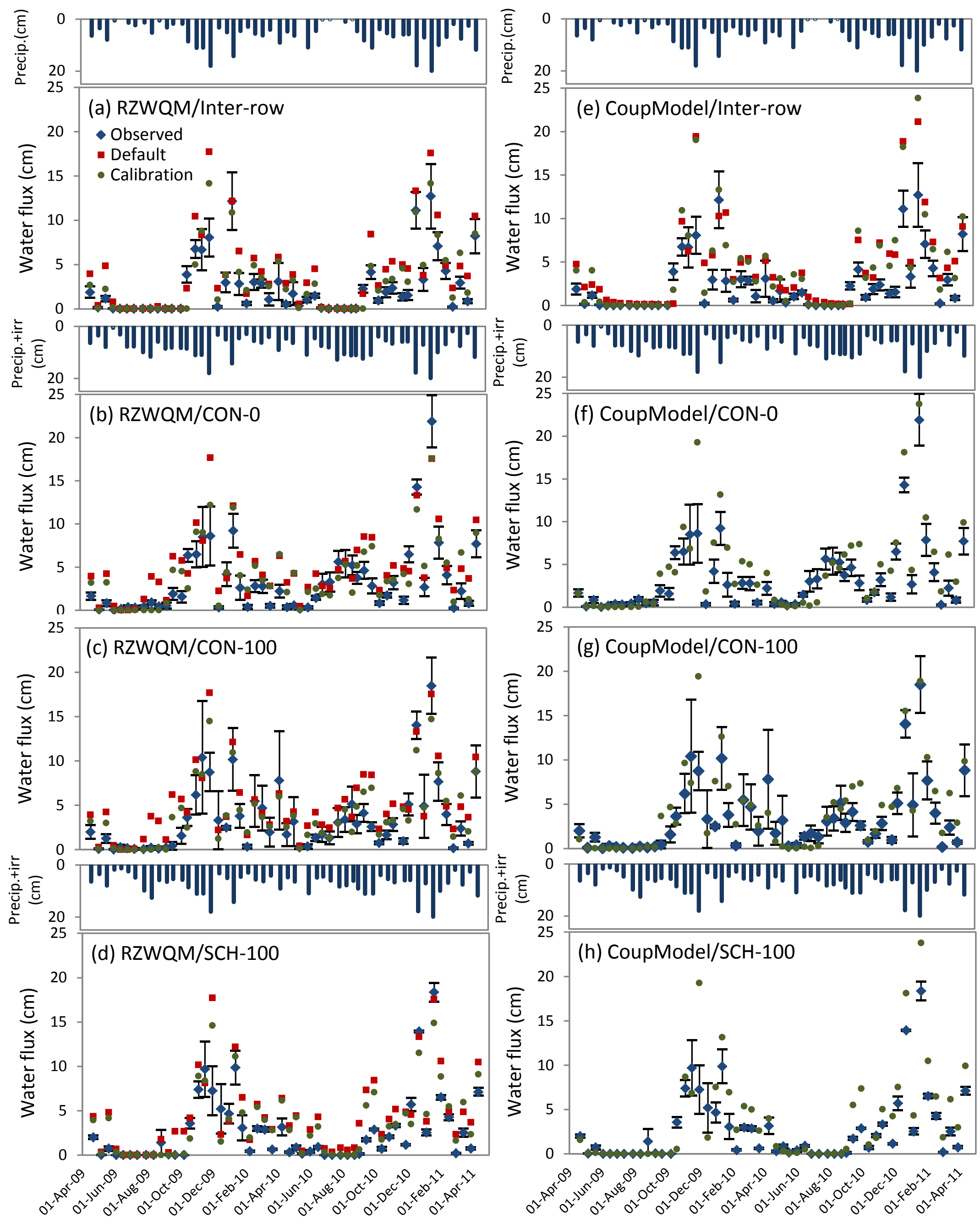

Figure 3.3: Comparison of observed and simulated water flux using default and calibrated parameters for the CoupModel and RZWQM. Water flux observation is the average (± standard deviation) PCAPS water data for four replicates. Precip. and irr. represent precipitation and irrigation, respectively.

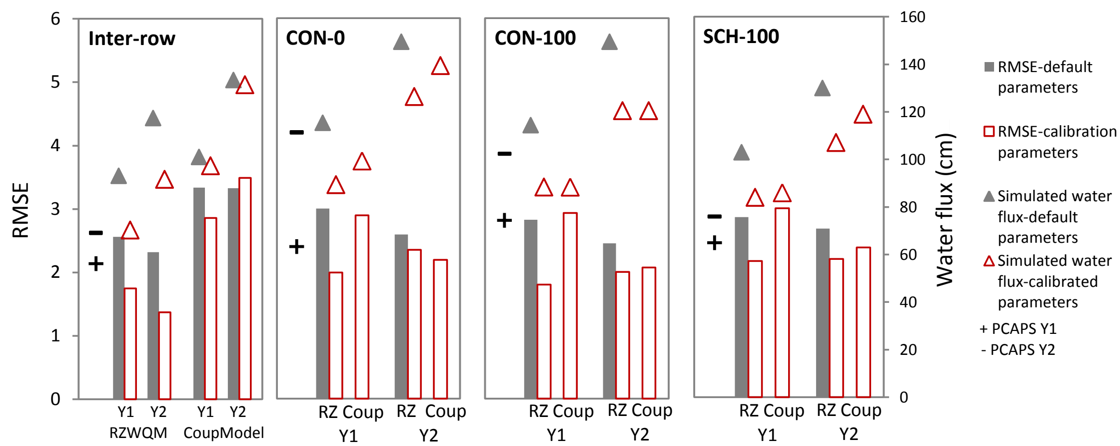

Figure 3.4: Comparison of the observed and simulated total water flux (using default and calibrated parameter sets) for Y1 and Y2, and evaluation of the performance of the models for this simulation.

imum and maximum RMSE of 2.81 and 2.98 cm. This suggests that the predicted water flux uncertainty for the CoupModel was small, and the model has a good consistency to reproduce measured data. The median of the CDF of the accepted outputs was used as the deterministic model prediction (Figure 3.3e). Calibrated hydraulic parameters were used to simulate water flux on raspberry rows in Y1. Maximum leaf conductance (g_{max}) was manually adjusted simultaneously for the three treatments to 0.025 m s^{-1} in Y1. Using the calibrated parameters, the water flux was simulated on the inter-rows and rows in Y2, and results were compared to the PCAPS water flux observations. Water flux estimations, using the calibrated parameters, were in reasonable agreement (with RMSE of 3.49, 2.19, 2.07 and 2.36 on the inter-rows and rows in treatments CON-0, CON-100 and SCH-100, respectively) with the PCAPS water flux observations for Y2 (Figure 3.4). Simulations with the calibrated hydraulic parameters reduced the RMSE compared to the default parameter set on the inter-rows for Y1 (14%); however, simulations with the default hydraulic parameters outperformed (5%) results from calibrated parameters during Y2 (Figure 3.4).

Water flux was overestimated using both the default and calibrated parameter sets for all treatments, ranging from 13 to 81% for the RZWQM and 17 to 91% for the CoupModel. These results are consistent with the findings of Kuchta (2012) who calculated water collection efficiency of the PCAPS. He concluded that the water collected by the PCAPS was less than expected drainage for the conventional (13 and 8% in Y1 and Y2, respectively) and scheduled (15 and 30% in Y1 and Y2, respectively) irrigation treatments. According to Kuchta (2012)'s calculations for the raspberry inter-rows, PCAPS water was 5% more and 19% less than expected drainage during Y1 and Y2.

For inter-rows, the calibrated RZWQM simulated water flux (RMSE of 1.75 and 1.37 in Y1 and Y2, respectively) better than the calibrated CoupModel (RMSE of 2.86 and 3.49 in Y1 and Y2, respectively). Also for the raspberry rows, the calibrated RZWQM outperformed the calibrated CoupModel (on average by 17% for Y1 and Y2 for three treatments), although an extra parameter, g_{max} which controls transpiration, was calibrated in addition to the soil hydraulic parameters for the CoupModel. This superior performance of the RZWQM is perhaps the result of a better calibrated model. That is, the GLUE algorithm with its random parameter sampling procedure did not calibrate the CoupModel as effective as DDS calibrated RZWQM. This assertion was corroborated by investigating the performance of the two algorithms to calibrate the nine hydraulic parameters in the RZWQM (Table 3.2). Calibrating the RZWQM using DDS outperformed (with RMSE of 2.2) simulation results obtained from calibration with the GLUE (with RMSE of 3.0) (Figure 3.5). This result is consistent with the findings of Tolson and Shoemaker (2008) who suggested that DDS-based uncertainty analysis methodology (DDS-AU) is hundreds or thousands of times more efficient at finding behavioral parameter sets than GLUE with random sampling. This finding suggests that the superior performance of the calibrated RZWQM can be related to the application of a better calibration method, and that the predictive capacity of the CoupModel was only within the limits of available calibration method for the CoupModel and the computational budget used (i.e., 5000 in this study). However, it is necessary to apply both algorithms to the CoupModel and compare the results to determine

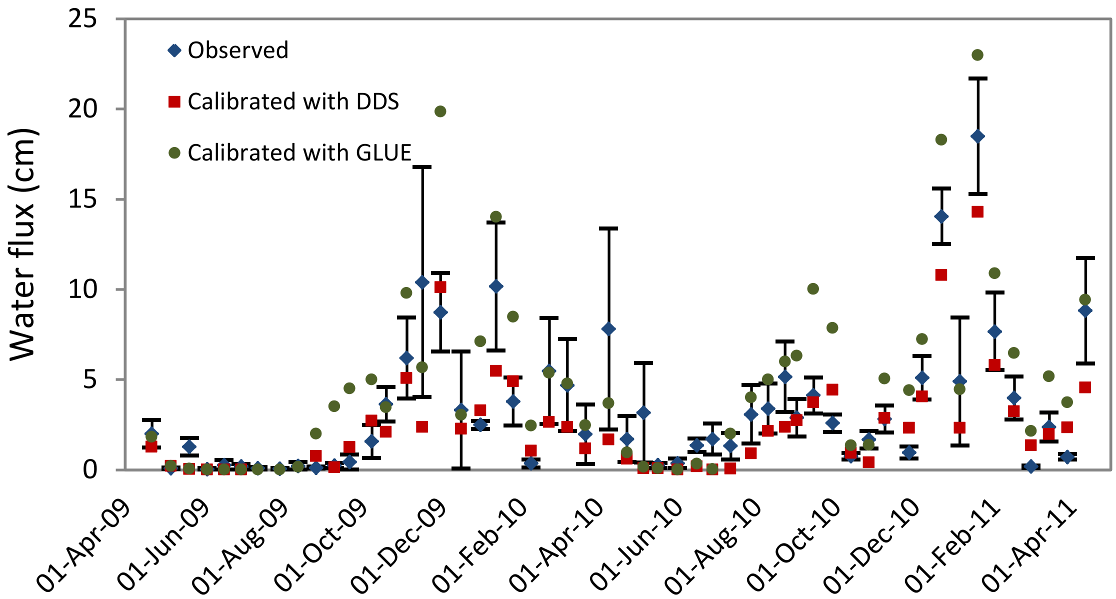

Figure 3.5: Comparison of the observed and simulated water flux time series using calibrated RZWQM for treatment CON-100. The DDS and the GLUE algorithms, each with 5000 model evaluations were used for the calibration. The RMSE for the model calibrated with DDS and GLUE was 2.2 and 3.0, respectively over the entire study period.

whether application of DDS could have resulted in a more effective calibration.

It is also noteworthy that the RZWQM simulated water flux using default hydraulic parameters significantly better than the CoupModel on the raspberry inter-rows (23 and 30% for Y1 and Y2) (Figure 3.4), meaning that the RZWQM was able to simulate water flux better than the CoupModel regardless of the calibration. Typically, input water in excess of run off, soil moisture capacity and ET moves to the depths below the root zone and into groundwater. In an attempt to uncover the difference between the performances of these two models for the simulation of water flow, processes related to soil water dynamics were compared. Both models used Brooks-Corey to describe soil hydraulic parameters and solve Richards' equation for water distribution. The effect of using the one-parameter and the full-parameter methods on RZWQM water flux estimation was investigated. Resulting water flux values from both Brooks-Corey methods are highly correlated (with R^2 of 91, 86, 84 and 84% for the inter-rows and the three treatments). This suggests that the difference between water flux estimation between the two models is not related to the method used to represent the soil moisture characteristic curve. Since both models predicted the total amount of run off of <5 cm in Y1 and Y2, the origin of the difference between these two models possibly lies in their ET estimation. The CoupModel implements the empirical Penman-Monteith equation (1965) which follows a single layer or big leaf approach with a single-bulk-surface resistance (including the stomatal and soil surface resistances) and single-aerodynamic resistance from the evaporating surface into the air above (Allen et al., 1998). Whereas, the extended model of Shuttleworth and Wallace (1985) which is implemented in the RZWQM, explicitly defines a partially covered soil, and predicts evaporation from the bare soil and residue-covered surface, and transpiration from the crop canopy (Farahani and Ahuja, 1996). The simulated ET by the two models for treatment CON-100 were compared to the atmometer ET measurements in Y1 and Y2 (Figure 3.6). Total ET measured by the atmometer was 372 mm for Y1 (May 05, 2009 to October 08, 2009) and 366 mm for Y2 (April 21, 2010 to October 01, 2010), respectively. For the same period in Y1 and Y2, the RZWQM estimated ET at 515 and 522 mm, whereas the CoupModel estimated ET at 555 and 588 mm, respectively. The correlation between field measurements and the RZWQM ET estimates (with R^2 of 65%) was higher than the correlation between measured and CoupModel ET estimates (with R^2 of 11%). This finding is consistent with Stannard (1993) who found that the Shuttleworth and Wallace method performs significantly better than Penman-Monteith equation for sparse crops. Together, the RZWQM simulates water flux comparatively better than the CoupModel due to the ET model employed.

Predicted water flux by both models reflects the total precipitation and irrigation pattern during the simulation period. Downward water flux occurs mostly from October to April as most precipitation (113 and 123 cm in Y1 and Y2) takes place over this period of time. Irrigation dominates infiltration from mid-spring to

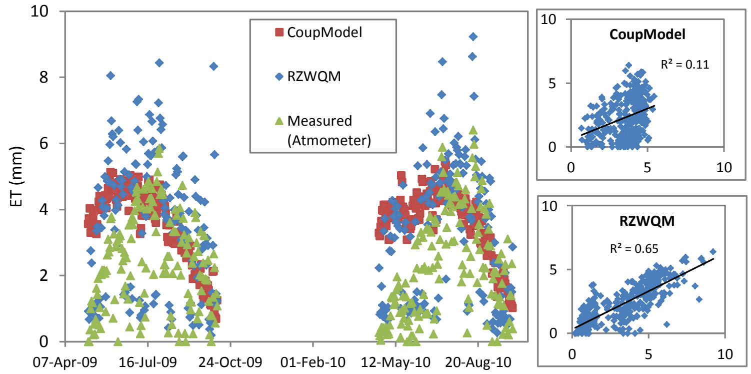

Figure 3.6: Comparison of ET simulated by the calibrated CoupModel and RZWQM. The CoupModel used empirical Penman-Monteith (1965) equation for simulating ET process; the RZWQM uses the extended model of Shuttleworth and Wallace (1985). Observed ET data were obtained from an atmometer.

late-summer particularly for CON-0 and CON-100 that were under the conventional irrigation practice. Except for September 2010 for which water flux was overestimated for all treatments (rows and inter-rows), both the RZWQM and CoupModel were able to well represent water flux over the study time period for the different treatments investigated (Figure 3.3).

The credibility of the calibrated hydraulic parameters for simulating water flux was also evaluated by comparing water flux estimates obtained from the calibrated (Table 3.3) and the field measured (Table 3.2) hydraulic parameters during Y1 and Y2. Measured hydraulic parameters, utilized for the simulation of the RZWQM with the one-parameter Brooks-Corey method included ρ_b, K_{sat} and FC, whereas for the CoupModel with the full brooks-Corey method these parameters were λ, ψ_b, θ_s, θ_r and K_{sat}. The correlation between observed and predicted water flux using calibrated (with R^2 of 74 to 85% for the RZWQM and 74 to 86% for the CoupModel) and measured (with R^2 of 71 to 86% for the RZWQM and 73 to 81% for the CoupModel) parameter sets are comparable (Figure 3.7). Moreover, the estimated water flux using the calibrated parameters has a slightly better correlation with PCAPS observations compared to the results using the measured parameter set.

Table 3.3: Calibrated soil hydraulic parameters. The DDS and GLUE optimization algorithms were used for the calibration of the RZWQM and the CoupModel. Values for the RZWQM represent the mean/standard deviation of the calibrated parameters obtained from the inter-rows and all three treatments in Y1. Values for the CoupModel were obtained from calibration for the inter-rows only.

Model	Soil layer	Parameter						
		λ	ψ_b	θ_s	θ_r	K_{sat}	FC	ρ_b
RZWQM	1	-	-	-	-	5.9/0.7	0.30/0	1.22/0
	2	-	-	-	-	1.34/0.0	0.26/0	1.42/0
	3	-	-	-	-	39.7/12	0.03/0	2.00/0
CoupModel	1	0.71	66	0.43	0.01	1.8	-	-
	2	0.33	52	0.39	0.01	3.8	-	-
	3	0.14	8	0.33	0.01	33.7	-	-

These findings determine the credibility of the calibrated hydraulic parameters in comparison to the field-measured values for simulating water flux below the root zone.

3.3.2 Calibration of SOM and Growth Parameters and Estimation of Nitrate Loading

The average nitrate loading, collected by the PCAPS, from the inter-rows was 47.7 and 59.5 kg ha^{-1} during Y1 and Y2, respectively. An amount of 8.6 kg ha^{-1} per year (Environment Canada, 1997) was deducted from these loading amounts to account for annual atmospheric deposition. The resulting values (39.1 and 50.9 kg ha^{-1}) were adopted as the average mineralized nitrogen for the inter-rows. Soil volumetric water content (VWC) on the inter-rows and rows under the three treatments was simulated during Y1 and Y2 irrigation seasons, using the RZWQM calibrated hydraulic parameters. The average soil VWC over the raspberry rows was 26%, whereas on the raspberry inter-rows, it was estimated as 20%. Using

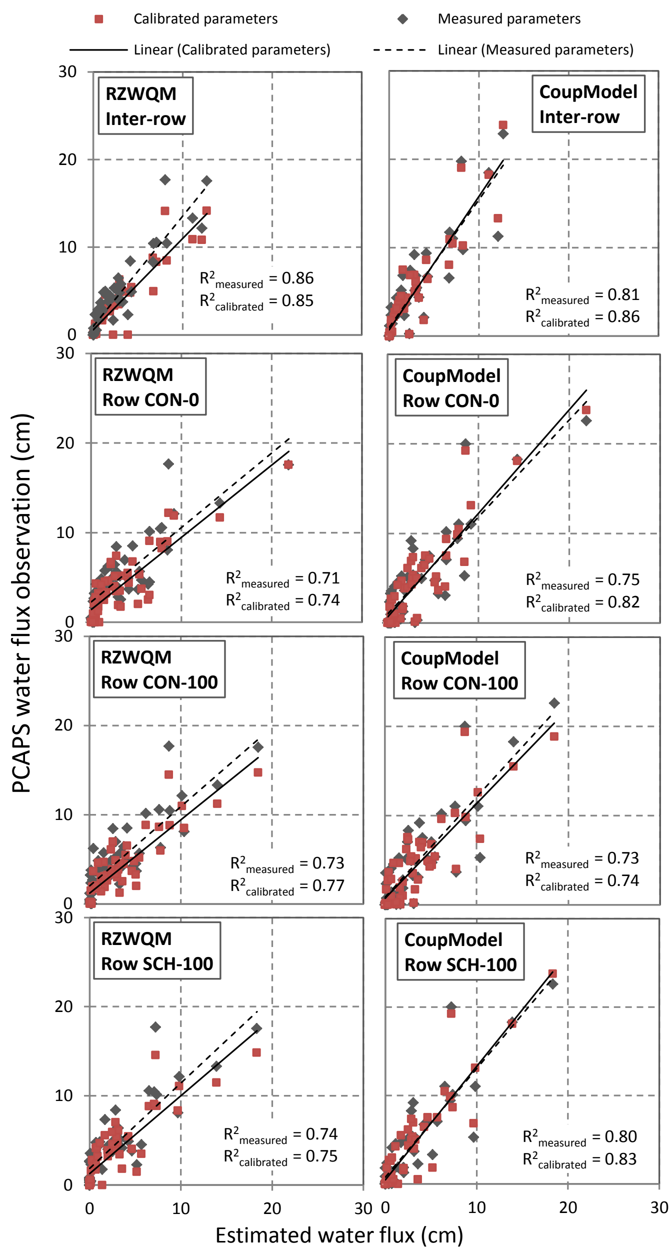

Figure 3.7: The relationship between PCAPS water flux observations and estimated water flux using laboratory-measured and calibrated hydraulic parameters in inter-rows and treatment rows CON-0, CON-100 and SCH-100 for the study period (April 2009 to April 2011). For RZWQM, ρ_b, K_{sat} and FC were used in the one-parameter Brooks and Corey method, whereas for the CoupModel the full Brooks and Corey parameter method using λ, ψ_b, θ_s, θ_r and K_{sat} was implemented.

Eq.(3.1), mineralization was adjusted for the raspberry rows during the irrigating seasons. As a result, the total amount of mineralized nitrogen during Y1 and Y2 for the raspberry rows was estimated at 49.5 and 62.1 kg ha^{-1}, respectively. SOM pool sizes and $t_{f \to int}$ were manually adjusted for the three treatments to obtain annual mineralization rates of 49.5 kg ha^{-1} and 62.1 kg ha^{-1} during Y1 and Y2, respectively, on the raspberry rows. SOM was partitioned between fast, intermediate and slow pools as 7, 13 and 80%, respectively. Also, $t_{f \to int}$ was calibrated to 0.65. The list of RZWQM parameters that were calibrated manually are given in Table 3.4. Finally, plant N-uptake was adjusted manually for the Y1 and Y2 growing season so that the simulated total nitrate loading matched the PCAPS nitrate loading for each year. It was assumed that excess soil nitrate during the growing season is leached from the soil profile generally before winter; therefore, plant N-uptake was modified using the PCAPS data from April 2009 to January 2010, and April 2010 to January 2011 for Y1 and Y2, respectively. Actual plant N-uptake was estimated as 66 and 53 kg ha^{-1} for treatment CON-0; 135 and 127 kg ha^{-1} for treatment CON-100; and 113 and 108 kg ha^{-1} for treatment SCH-100 during Y1 and Y2 growing seasons, respectively.

The SOM parameters and seasonal plant N-uptake for the RZWQM were calibrated using seasonal nitrate loss during Y1 and Y2. A concern was how the RZWQM would simulate temporal fluctuations of nitrate loading if these calibrated parameters were available. To address this concern, simulated nitrate loading time series using all calibrated parameters were compared to the PCAPS nitrate data (Figure 3.8). The calibrated RZWQM represented the PCAPS loading nitrate time series with a RMSE of 19 μg N cm^{-2} on inter-rows and 42, 34, and 51 μg N cm^{-2} on treatments CON-0, CON-100 and SCH-100, respectively during the entire study period (Figure 3.9). The calibrated RZWQM does not represent the PCAPS nitrate loading data time series in Y2 (with RMSE of 30, 20 and 38 μg N cm^{-2} for treatments CON-0, Con-100 and SCH-100) as well as Y1 (with RMSE of 17, 18, 28 μg N cm^{-2} for treatments CON-0, Con-100 and SCH-100). Also, the peak of simulated nitrate loading in Y2 has a lag time of about one month for treatments

Table 3.4: Manually calibrated SOM and raspberry growth and potential N-uptake parameters for the RZWQM and the CoupModel.

Model	Parameter	Unit	Default	Calibrated
RZWQM	$t_{f \to int}$	-	0.6	0.65
	Fast pool size	%	-	7
	Intermediate pool size	%	-	13
	Slow pool size	%	-	80
	Seasonal N-uptake (for CON-0)	kg ha^{-1}	100	107/74
	Seasonal N-uptake (for CON-100)	kg ha^{-1}	100	195/173
	Seasonal N-uptake (for SCH-100)	kg ha^{-1}	100	141/119
CoupModel	g_{max}	m s^{-1}	0.02	0.025
	$f_{e,l}$	Day^{-1}	0.5	0.6
	$f_{e,h}$	Day^{-1}	0.5	0.5
	k_l	Day^{-1}	0.035	0.03
	k_h	Day^{-1}	5E-005	5E-005
	${p_{ua}}^{(1)}$ (for CON-0)	gm^{-2}yr^{-1}	20	28/23
	${p_{ua}}^{(1)}$ (for CON-100)	gm^{-2}yr^{-1}	20	55/45
	${p_{ua}}^{(1)}$ (for SCH-100)	gm^{-2}yr^{-1}	20	30/25
	${p_{ub}}^{(1)}$	-	1	0.8
	${p_{uc}}^{(1)}$	Day^{-1}	0.12	0.6
	${cn_p}^{(1)}$	-	25	30
	${\varepsilon_w}^{(2)}$ (for CON-0)	g Dwmm^{-1}	3	5.4/4.6
	${\varepsilon_w}^{(2)}$ (for CON-100)	g Dwmm^{-1}	3	6.1/5.7
	${\varepsilon_w}^{(2)}$ (for SCH-100)	g Dwmm^{-1}	3	4.7/4.3

(1) Parameters associated with the logistic growth approach in the CoupModel; (2) Parameters associated with the WUE approach in the CoupModel. The seasonal N-uptake, p_{ua} and ε_w were calibrated for Y1/Y2.

CON-0 and CON-100 compared with the PCAPS observations (Figure 3.8). Moreover, the calibrated RZWQM underestimated nitrate loading during winter and spring (mid-December to mid-April) of Y1 (72, 59, 76 and 84% for the inter-rows and rows under treatments CON-0, Con-100 and SCH-100) and Y2 (78, 85, 91, and 93% for the inter-rows and rows under treatments CON-0, Con-100 and SCH-100) (Figure 3.10). Nitrate loss during this period of time is most likely related to the background mineralization of SOM. Overall the trends in nitrate loading were reproduced rather well with the calibrated RZWQM but the finer details are missing or only partially captured.

Selected SOM parameters for the CoupModel including $f_{e,l}$, $f_{e,h}$, k_l and k_h were manually calibrated for the inter-rows to 0.6, 0.5, 0.03 and 5×10^{-5} day^{-1}, respectively (Table 3.4). Calibrated hydraulic and soil organic parameters were used in the CoupModel to simulate plant growth on the raspberry rows. For the logistic growth approach, p_{ub}, p_{uc} and cn_p were simultaneously adjusted for all treatments to 0.8, 0.6 and 30, whereas p_{ua} was calibrated for each treatment for Y1 and Y2, separately (Table 3.4). PCAPS nitrate loading data from April 2009 to January 2010 and from April 2010 to January 2011 were used as the observation data to calibrate the logistic growth parameters for Y1 and Y2, respectively. As a result, the actual seasonal N-uptake were estimated as 51 and 45 kg ha^{-1} for treatment CON-0; 128 and 123 kg ha^{-1} for treatment CON-100; and 108 and 99 kg ha^{-1} for treatment SCH-100 in the growing seasons of Y1 and Y2, respectively. For the WUE approach, ε_w (μg CO_2 mmol^{-1} H_2O^{-1}) was adjusted to 5.4 and 4.6 for treatment CON-0; 6.1 and 5.7 for treatment CON-100; and 4.7 and 4.3 for treatment SCH-100 for the growing seasons of Y1 and Y2, respectively. The ε_w is known to be relatively constant for a given crop under a given climate condition (Hanks, 1983), regardless of the quantity of water supply (de Wit, 1958); therefore according to the results of this calibration, an average value of 5.13 (μg CO_2 mmol^{-1} H_2O^{-1}) is proposed for raspberry crops under the current climate conditions. For the WUE method, actual plant N-uptake was estimated at 54 and 46 kg ha^{-1} for treatment CON-0, 120 and 126 kg ha^{-1} for treatment CON-100, and 104 and 96

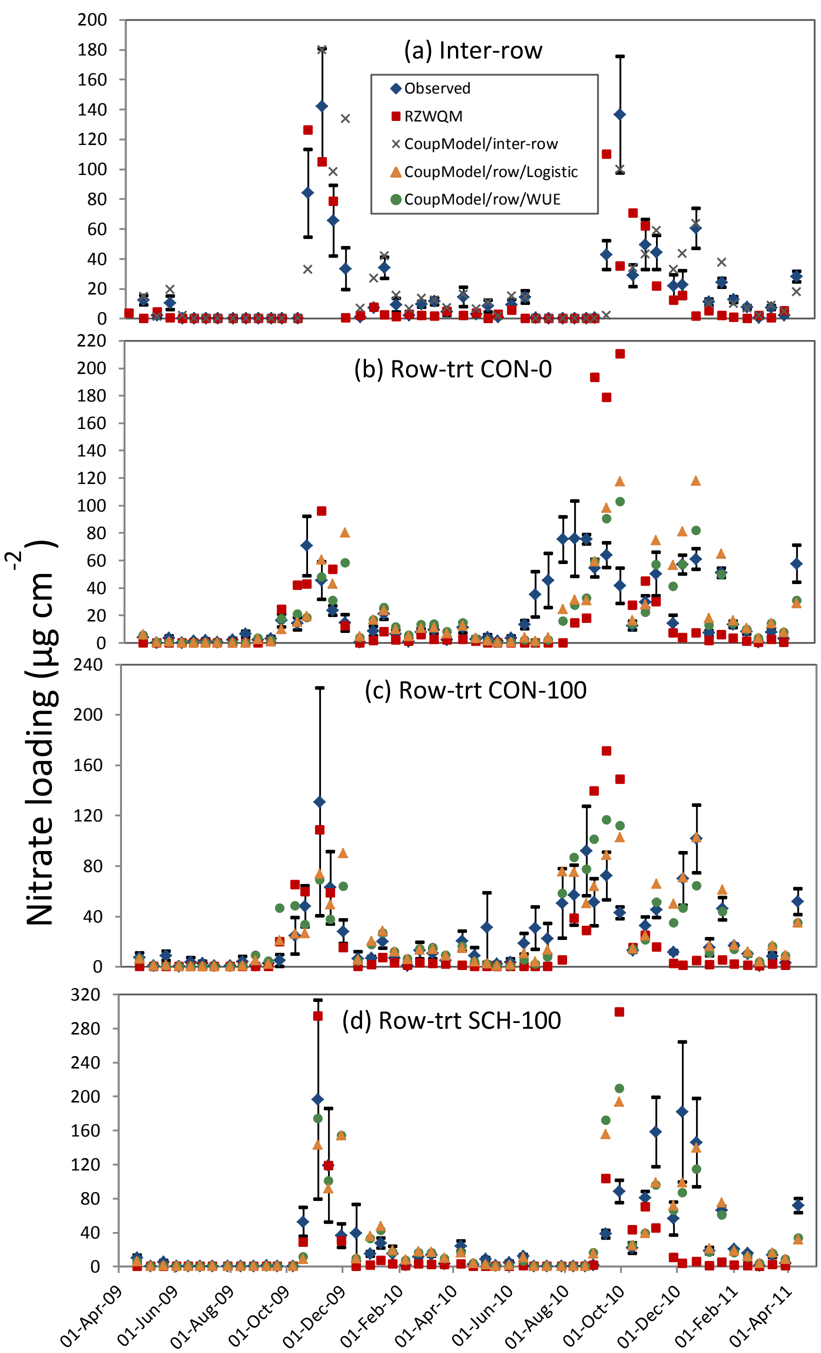

Figure 3.8: Observed and simulated nitrate loading with calibrated hydraulic, SOM and N-uptake parameters for CoupModel and RZWQM. Nitrate loading observation is the average (±standard deviation) PCAPS nitrate data from four replicates.

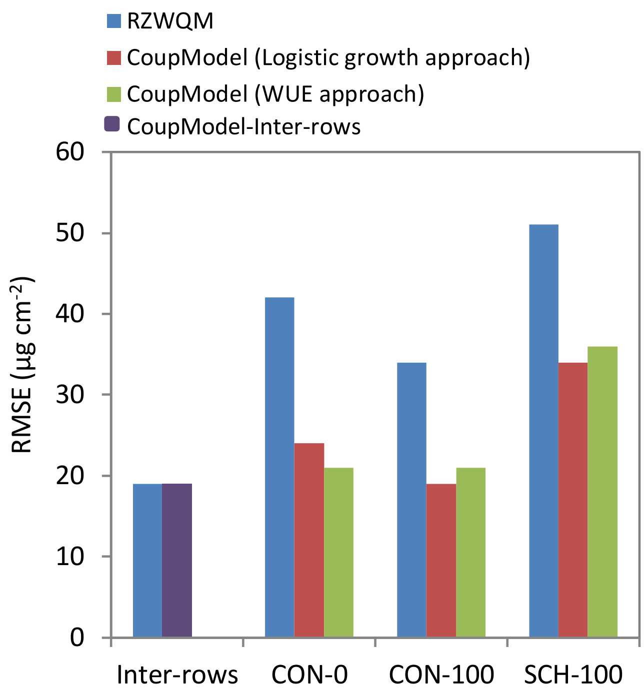

Figure 3.9: Evaluation of the performances of the RZWQM and the CoupModel for simulating nitrate loading for the entire study period using all calibrated parameters.

kg ha^{-1} for treatment SCH-100 during growing seasons of Y1 and Y2, respectively.

Temporal fluctuations of the simulated nitrate loading, using all calibrated parameters, was compared to the PCAPS nitrate data (Figure 3.8). Unlike the RZWQM, the CoupModel overestimated simulated soil background mineralization during winter and spring of Y1 and Y2 for the inter-rows and under rows for most treatments, using both growth approaches; however, with less error (Figure 3.8 and Figure 3.10). As depicted in Figure 3.8, similar to RZWQM, there was a lag time between the observed and estimated peak nitrate loading for treatment CON-0 in 2010, using the two growth approaches of the CoupModel; however, the magnitude of this error was less than that for RZWQM. The simulated nitrate loading time series was similar to the PCAPS nitrate fluctuations for the entire simulation period (Figure 3.8). The RMSE was 24, 19, 34 and μg N cm^{-2} for treatments CON-0, CON-100 and SCH-100, respectively, for the logistic growth approach, and 21, 21,

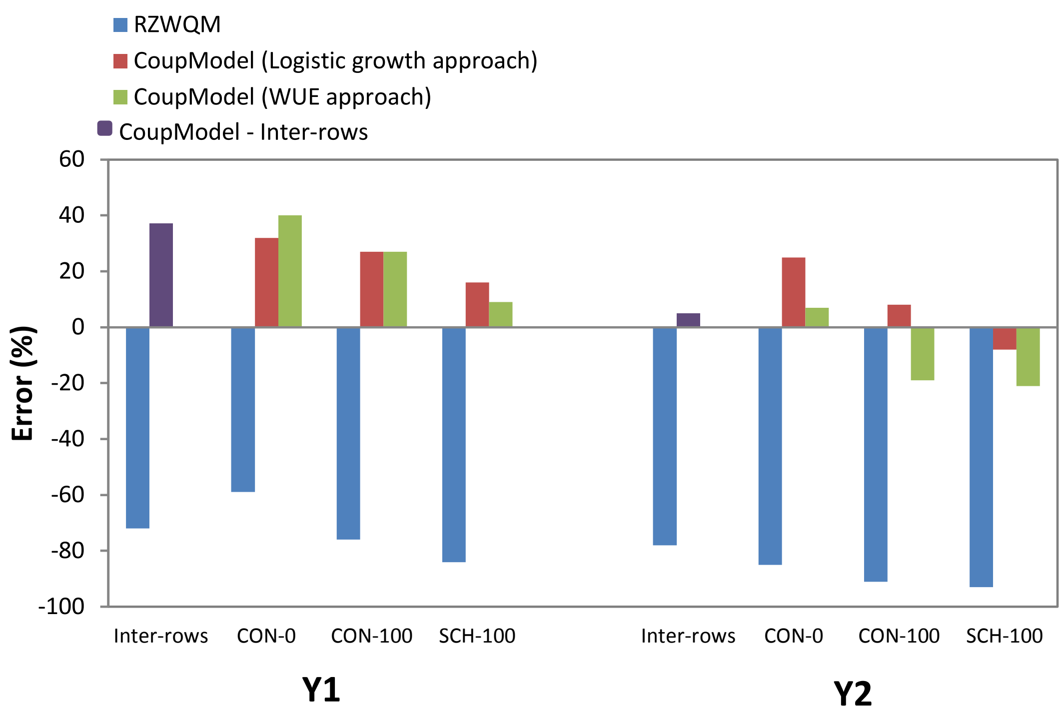

Figure 3.10: Total nitrate loading estimated for winter and spring (mid-December to mid-April) of Y1 and Y2. Positive values represent overestimation, and negative values represent underestimation.

and 36 μg N cm^{-2} for treatments CON-0, CON-100 and SCH-100, respectively, for the WUE approach. Also the RMSE for the inter-rows was 19 μg N cm^{-2}.

By comparing the water and nitrate flux time series (Figure 3.3 and Figure 3.8) it is clear that the temporal distribution of nitrate loading is highly correlated with water flux for both the RZWQM and CoupModel. In particular, the overestimation of nitrate loading coincides with the overestimation of water flux in September 2010 for treatment SCH-100. This correlation between water flux and nitrate loading time series is related to high permeability of the soil profile, and suggests that errors in water flux simulation can be transferred to the nitrate loading simulation. In this study, the CoupModel simulated water flux less well compared to the RZWQM; however, based on RMSE values the CoupModel outperforms the RZWQM for simulating nitrate loading on all raspberry treatments (Figure 3.9). The less well performance of the RZWQM can be attributed to the use of a simplistic model by the RZWQM to mimic the effect of perennial woody species such as raspberry on nitrate loss. Also, it is possible that calibration of plant growth parameters compensated for uncertainties and errors assiciated with water flux simulation in a way that nitrate loading simulation by the CoupModel even outperformed RZWQM results.

Estimated N-uptake in treatment CON-0 was rather significant considering that this treatment received no fertilizer. Mineralization of SOM and nitrogen addition in irrigation water are believed to be the main sources for N-uptake in treatment CON-0. Also, the decrease in the plant N-uptake (15%) in the second growing season for this treatment was likely related to the exhaustion of the mineralizable nitrogen pool.

According to the model estimations, 100 kg N ha^{-1} fertilizer application in treatments CON-100 and SCH-100 resulted in 74 and 52 kg ha^{-1} increases in plant N-uptake in each growing season when compared to treatment CON-0 with zero fertilizer application. This means that apparent fertilizer N recovery in treatment CON-100 was 74%. The difference between N-uptake in treatments CON-100 and SCH-100 (i.e., 22 kg ha^{-1}) was related to the irrigation nitrogen background added due to the difference between conventional and scheduled irrigation practices in these treatments. This means that the fertilizer-use efficiency in treatment SCH-100 is similar to the CON-100. Also, it was estimated that 20 and 17 kg ha^{-1} of the applied fertilizer was lost by volatilization in treatments CON-100 and SCH-100, respectively.

3.4 Conclusion

The main objective of this study was to evaluate the performance of RZWQM and CoupModel to simulate water flux and nitrate loading below the raspberry root zone. A step-by-step approach was developed based on available field observations on raspberry rows and inter-rows not only to calibrate the selected soil hydraulic, organic matter and growth parameters of each model, but also to define two import nitrogen source (i.e., mineralization) and sink (i.e., N-uptake) terms in the soil nitrogen budget.

Water flux simulation improved by 37% for the RZWQM when calibrated hydraulic parameters replaced the model default values. This suggests that the calibration was effective and is worth the time and effort. However, for the CoupModel, calibration of the soil hydraulic parameters did not consistently improve the performance of the model for simulating water flux during the calibration and validation period, and hence, based on the findings of this study, default and calibrated soil hydraulic parameter sets can be used interchangeably.

The calibrated RZWQM and CoupModel both simulated water flux well; however, the calibrated RZWQM (RMSE 1.98 cm) outperformed the CoupModel (RMSE 2.53 cm) over the validation period (i.e., Y2). It was found that the outperformance of the RZWQM is partially related to the application of a more efficient calibration algorithm (i.e., DDS). The RZWQM, also, considerably outperformed the CoupModel to simulate water flux before calibration using the default soil hydraulic parameters. This was found to be related to the application of a better ET model in the RZWQM.

The calibrated CoupModel simulated the nitrate loading time series better than RZWQM (on average by 34% for inter-rows and all treatments) using both logistic and WUE growth models. Due to the high permeability of the study site, nitrate loading fluctuations were greatly correlated with water flux amount and timing, suggesting the error associated with water flux estimation can easily be transferred to the nitrate loading simulations. This was not consistent with the overall findings of this study that the CoupModel simulated water flux less well compared to the RZWQM, while it outperforms RZWQM for simulating nitrate loading. It was likely that calibrating growth parameters of the CoupModel had overridden the effect of water flux simulation error, and resulted in better simulation of nitrate loading.

This effect, however, should be carefully watched when multi-processes models such as CoupModel are calibrated since it may result in over-parameterization of the model and deteriorates the robustness of the calibration.

Plant N-uptake is normally a dominant sink term in cropped systems. The findings in this study indicate that the plant N-uptake is sensitive to the agricultural management practice, and small changes of this parameter have great influence on soil nitrogen level. Therefore, one single value does not represent all conditions, and parameterization of this parameter is critical when the RZWQM and CoupModel with the logistic growth approach are used. However, the WUE growth approach in the CoupModel with only one parameter, ε_w which is constant for a specific plant and climate condition is more robust for a reliable predictions. Under the current study conditions, an average value of 5.13 (μg CO_2 mmol^{-1} H_2O^{-1}) was obtained for ε_w for raspberry crop.

Overall, information about SOM and growth parameters is vital for reliable application of both models. With such information, the CoupModel and the RZWQM (to a lesser extent) were found to be reliable tools to simulate nitrate loading to the groundwater. It is expected that better calibration of soil hydraulic parameters and more characterization of plant development and carbon allocation parameters will improve the CoupModel predictions. For the RZWQM, an inclusive growth model needs to become available for the simulation of woody species such as raspberry to obtain better nitrate loading estimations.

Chapter 4

Simulation of water and nitrate fluxes for similar agricultural systems: transportability of model parameters within a landscape

Outline

Being a non-point source pollutant, nitrate leaching usually needs to be evaluated at various locations over an aquifer to integrate agricultural impact on groundwater quality and to develop strategies that mitigate contamination. Because required field data are not usually available for every different location within an agricultural landscape, models are considered as potentially useful tools for such investigations. Using models, however, is usually associated with significant data and calibration requirements. A transportable model that is able to simulate nitrate leaching in other locations with relevant environmental variables is a useful tool to evaluate agricultural impact on groundwater quality, particularly for the distant areas with poor possibility of field assessment and model calibration. In this study, the applicability of the agricultural system model, CoupModel, which was previously calibrated and successfully validated for predicting water and nitrate fluxes below the raspberry root zone, was investigated in a conventional raspberry farm, located 2 km away from the calibrating site within the Abbotsford physiographic region in south western BC, Canada. The transported CoupModel overestimated water flux by 24% for the conventional raspberry farm; however, replacing the transported hydraulic parameters by the locally-measured parameter values of the conventional raspberry farm did not reduce the error. Simulation of nitrate flux using transported model was associated with significant error of 104%, but application of the locally-measured hydraulic parameters reduced this error only by 17%. This means that the locally measured hydraulic parameters do not prevail over the transported parameter values, and can be replaced by them if local measurements are not available. By adopting the concept of similar media and using single value scaling factor method, soil hydraulic parameters were scaled to the farm level, and were used to integrate water and nitrate flux simulations. The variability of soil hydraulic parameters across the farm had little effect on the annual water flux simulation, but influenced nitrate flux simulations by up to 28% for the year in which manure is applied to the farm, suggesting that the mineralization of organic manure is sensitive to the variability of soil hydraulic parameters. In general, transported hydraulic parameters were found to be as applicable for simulating water flow and nitrate flux beneath the conventional farm as the locally measured parameters (except for the year in which manure was applied). Further sampling, modeling, and validation at additional field sites with different management practices are required to properly confirm CoupModel transportability within the Abbotsford physiographic region.

4.1 Introduction

Underlying the lower Fraser Valley in south western British Columbia, Canada and the Nooksack lowlands in northern Washington State, USA is the shallow uncon-

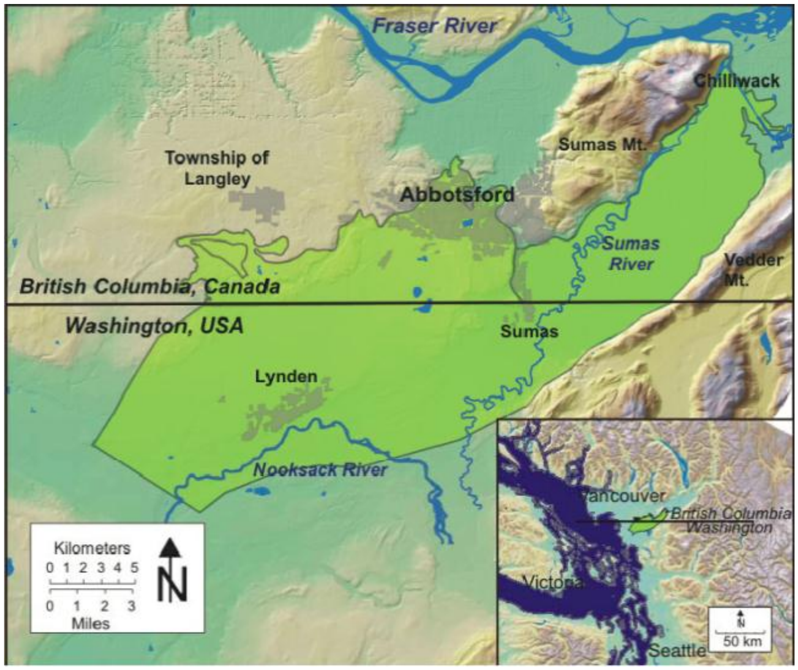

Figure 4.1: Location of the Abbotsford-Sumas Aquifer in the Central Fraser Valley (Adopted from Allen et al. (2008)).

fined Abbotsford-Sumas Aquifer which supplies water for nearly 100 000 people in Canada and 10 000 people in the United States (Mitchell et al., 2003) (Figure 4.1). The lower Fraser Valley is an intensive farming region, with raspberries being the predominant crop above the Canadian portion of the aquifer (Hii et al., 1999). Nutrient application practices associated with raspberry production have been identified as the significant contributor to nitrate contamination of the aquifer (Mitchell et al., 2003; Zebarth et al., 1998; Wassenaar, 1995).

The aquifer is comprised of predominantly heterogeneous sand and gravel deposits of glaciofluvial drift origin (Armstrong et al., 1965), and the surficial soil layer is well-drained due to its sandy texture. As a result, residual nitrate in the shallow soil profile after the growing season is completely leached from the vadose-zone and arrives at the water table in three months (Chesnaux and Allen, 2008). Also, surplus nitrogen fertilizer, if applied in April, is thoroughly leached into the groundwater in seven months (Chesnaux et al., 2007). These findings emphasize the need to investigate the magnitude and timing of nitrate formation and subsequent leaching from the root zone.

Agricultural models are useful tools to understand soil nitrogen processes within the root zone, and to explore various agricultural management strategies. Although, many studies have been conducted to understand the sources of nitrogen, and to quantify the formation and transport of nitrate to the Abbotsford-Sumas aquifer (Wassenaar et al., 2006; Zebarth et al., 2002, 1999; Dean et al., 2000; Zebarth et al., 1998; Wassenaar, 1995; Zebarth et al., 1995), the role of models in these investigations has been minor. Chesnaux and Allen (2008) and Chesnaux et al. (2007) used a water seepage model (SEEP/W) and a contaminant transport model (CTRAN/W) to simulate nitrate transport in the vadose-zone. In the study conducted by Chesnaux and Allen (2008), an average residual nitrate concentration, measured after the growing season, over a four-year survey period was used as the leachable nitrogen in the transport simulations. Chesnaux et al. (2007) used an annual nitrogen balance approach, based on soil nitrogen inputs and outputs, to approximate available nitrate for leaching. As mentioned by Chesnaux et al. (2007), the net nitrogen approach and the one-time soil nitrate measurement method, used to estimate leachable nitrate in these studies, only represent an approximation of actual conditions. That is, processes that control leachable nitrate are time-dependant, and hence leachable nitrate is time-variant. Therefore, in the efforts of Chesnaux et al. (2007) and Chesnaux and Allen (2008), transport of nitrate was simulated only for a one-pulse event (not over time). Agricultural system models can account for the variation of the processes that influence soil nitrate concentration over time, and hence can provide more reliable estimates for leaching nitrate from the root zone. Simulated leachable nitrate may replace field measurements and annual nitrogen balance approximations for vadose-zone modelling.

Parameter calibration is often necessary for a successful model application. The common cost of model calibration includes thousands of model evaluations and having enough field observations which are likely only affordable in research-level studies. The act of calibration adapts the model to particular situations. As a result, the calibrated parameters contain information about the conditions (such as soil, crop type, agricultural practice and climate) of the site and temporal period over which the data were gathered. It is common to test the predictive capability of the calibrated model for a period other than the calibration period, so-called model validation (Refsgaard, 2001). It adds to the value of a calibrated model if the model is proved to be transportable; i.e., be able to simulate nitrate leaching in other local or regional locations with relevant environmental variables. This capability is particularly of interest when considering the fact that nitrate is a non-point source pollutant and it often needs to be evaluated at different locations within a landscape to integrate agricultural impact on groundwater quality. Transportable models are especially useful for the distant areas with high cost or poor possibility of field assessment of nitrate leaching but strong contribution to the aquifer contamination.

The CoupModel (Jansson and Karlberg, 2012) is a detailed research-level agricultural system model (Shaffer, 2002) that features complex soil hydrological and nitrogen cycle processes for cropped systems. In one recent study (see Chapter 3), the ability of the CoupModel to simulate water flux and nitrogen leaching from the raspberry root zone was investigated using a set of field data obtained from an experimental field located over the Abbotsford-Sumas Aquifer. The investigation included different agricultural management scenarios. One of the studied practices included the grower's common practice which resembles conventional raspberry farms in the Abbotsford region. Selected hydraulic, organic matter and crop growth parameters were calibrated, and successfully validated against observed water flux and nitrate leaching data.

The main objective of this study was to investigate the transportability of the calibrated CoupModel to a conventional raspberry farm, located 2 km in northwest of the calibration field, located within the Abbotsford region, to simulate water and nitrate flux below the root zone. According to the soil survey of the Lower Fraser Valley (Ministry of Environment, British Columbia, 1980), more than 1000 ha of the agricultural lands in the Abbotsford region is dominated by conventional raspberry production. These agricultural parcels, in general, share common climate conditions, soil properties and cropping management. Therefore, results of this study are expected to be useful to investigate nitrate leaching from this physiographic region into the Aquifer.

This study contains two sections: In the first section, the calibrated CoupModel ("transported model") from the experimental raspberry field ("calibrating site") was used to simulate water and nitrate fluxes from the conventional raspberry farm. These simulation results were compared to the field estimates, collected from May 2010 to March 2011, to examine the applicability of the transported model. Also, the predictive ability of the transported model if the hydraulic parameters of the transported model are replaced with the local hydraulic parameter, measured for the conventional farm, was investigated. The goal was to investigate whether locally-measured parameters can improve CoupModel simulations compared to the transported parameters. For this effort, no field-measured or locally-calibrated quantities were available to use for soil organic matter (SOM) and growth parameters.

In the second section, soil hydraulic parameters were scaled to the farm level with an area of 15 ha using a scaling factor method, and were then used to simulate annual water and nitrate fluxes, integrated for the entire conventional farm, over a four-year period from 2007 to 2010. Simulation results were compared to those obtained from using the transported and measured hydraulic parameters to investigate whether 1) measured parameters can represent spatial variability across the conventional farm, and 2) transported parameters can be used as a substitute for the scaled hydraulic parameters to simulate water and nitrate fluxes for the conventional farm. This long-term simulation survey, includes a range of various types and amounts of nitrogen applications and climate conditions, and hence, is expected to provide a thorough comparison of the application of different sets of hydraulic parameters.

4.2 Materials and Methods

4.2.1 Site Description

In this section, the environmental conditions and agricultural management practices of the conventional raspberry farm are described, and compared to those of the calibrating site. The calibrating site is particularly related to the experimental treatment which was designed to represent the conventional farming practice.

Climate. The Abbotsford Airport weather station (Environment Canada, 2012a) represents the weather conditions of both the calibrating site and the conventional raspberry farm. The average annual precipitation at this station is 1570 mm, and the average monthly temperature ranges from 2.6 °C in January to 17.7 °C in August with an annual average of 10.0 °C. The annual precipitation in the study period comprising 2007 to 2010 was 1687, 1233, 1387 and 1495 mm, respectively.

Soil. According to the soil map of the Lower Fraser Valley (Ministry of Environment, British Columbia, 1980) the soil at the conventional raspberry farm was defined as Abbotsford, whereas soil at the calibrating site is categorized as Marble Hill. The general characteristics of both soils are similar; that is, a 20-50 cm thick layer (for the Marble Hill soil, more than 50 cm) of medium-textured eolian deposits over a gravelly glacial outwash (non to moderately stony and very gently sloping). At both sites, the transition from eolian soil to loose sand gravel soil occurs with a sharp interface. Detailed soil information for the upper 1 m of the soil profile is in Table 4.1. At both sites, the soil profile consists of three soil layers including two loam layers with different hydraulic properties which lie on an extremely sandy soil layer, identified as the top of the aquifer. At the conventional farm, soil was elevated for 15 to 20 cm on the raspberry rows. As a result, the thickness of the top soil, which is identified as the agricultural soil, at the conventional farm was greater than at the calibrating site.

Farming Practices. Both sites were under raspberry (*Rubus ideaus* L.) crop farming. Raspberries are perennial crops. They remain in production usually for

Table 4.1: Soil horizon information based on the field survey and laboratory characterization for the calibrating site and the conventional raspberry farm.

Depth (cm)	Index	Soil classification and texture	Gravel (%)	Sand (%)	Silt & Clay (%)
Calibrating site					
0-25	Layer 1 (L1)	Loam	4	26	70
25-60	Layer 2 (L2)	Loam	5	31	64
60-100	Layer 3 (L3)	Sand	30	64	0
Conventional farm					
0-45	Layer 1 (L1)	Loam	2	36	62
45-60	Layer 2 (L2)	Sandy loam	5	77	18
60-100	Layer 3 (L3)	Sand	4	93	3

5 to 15 years, depending on the vigor of the crop, and removed after this period of time for soil rejuvenation and new plantation. In the conventional raspberry farm, raspberries were planted in spring 2007, whereas in the calibrating site, plantation took place in November 2008. Raspberry crops are usually planted in rows to accommodate tractor operations. At both study sites the rows are spaced 3 m apart. A 1.2 m wide "herbicide strip", centered on the crop row, was maintained vegetation-free at both sites. It is common to establish cover crops between raspberry rows. At the conventional raspberry farm, barley was seeded between rows in September, and was tilled in early spring. At the calibrating site, the inter-rows were clean-cultivated. Production, maintenance and pest management activities at the calibrating site were standardized according to the BC Berry Production Guide (British Columbia Ministry of Agriculture and Lands, 2009), and was assumed to be followed at the conventional farm. Each fall, raspberry canes from the previous year were pruned, left in the inter-rows, and mowed in the next spring at both sites.

The irrigation practice at the conventional farm included drip irrigation (30 cm emitter spacing with 2 L h^{-1} discharge). The irrigation schedule was not available. Based on general information of the growers' common practice for raspberry farms, it was assumed that irrigation took place every other day starting June 10 and stopping September 20 each year, with 4 h day^{-1} irrigation during July 10 to August 20, and 2 h day^{-1} for the rest of the irrigation season to avoid the risk of root rot. As a result, 90 cm of water was delivered to the crops every growing season. The irrigation practice in the calibrating site included 71 and 80 cm drip irrigation in the growing seasons of 2009 and 2010. Groundwater was the source of irrigating water which contains 16.5 and 0.03 mg L^{-1} nitrate and ammonium.

At the conventional raspberry farm, 64 m^{3}ha^{-1} manure was applied before planting in spring 2007. The type and characteristics of the applied manure are not known. Poultry production is common across the Abbotsford region. Accordingly, it was assumed that the applied manure was poultry broiler litter with a C:N ratio of 15, bulk density of 330 kg m^{-3} and 25% moisture content (Alberta Agriculture and Rural Development, 2012). As a result, this manure application is equivalent to 744.5 kg ha^{-1} of nitrogen. At the conventional farm, the synthetic nitrogen was applied at the rate of 24 and 34 kg ha^{-1} in 2009. The first nitrogen fertilizer split in 2009 was lower because cane growth appeared overly vigorous in 2008. In 2010, two splits of 34 kg ha^{-1} of nitrogen were applied in April and May. At the calibrating site, two splits of 50 kg ha^{-1} fertilizer were applied in April and May of 2009 and 2010 (Table 4.2).

4.2.2 Data Collection Effort

A field experiment was conducted at the conventional farm to collect soil water and nitrate transport data with the purpose of model evaluation. Detailed physical and hydraulic properties of each soil layer were investigated at this location ("locally-measured"). These included soil fractions (ASTM D69-04, 2009) (Table 4.1), and the relationship between soil moisture and pressure, known as soil moisture retention curve (SMRC) by using the pressure plate method (ASTM C1699-09, 2009; Richards, 1948, 1965) (Figure 4.2). Daily soil water content was recorded at depths of 20, 35, 52 and 70 cm on the raspberry row, using 5TE Sensors (Decogon De-

Table 4.2: Farming practices at the calibrating site and the conventional raspberry farm.

	Conventional farm	Calibrating site
Plantation	Spring 2007	November 2008
Row spacing	3 m	3 m
Cover crop	barley	None
Irrigation	Drip (90 cm per year)	Drip (71 cm for 2009 and 80 cm in 2010)
Irrigation nitrogen background	16.5 mg $NO_3^- - N\ L^{-1}$ 0.03 mg $NH_4^+ - N\ L^{-1}$	16.5 mg $NO_3^- - N\ L^{-1}$ 0.03 mg $NH_4^+ - N\ L^{-1}$
Manure N	744.5 kg ha^{-1}	-
Fertilizer N (urea)	None in 2007 and 2008 58 kg ha^{-1} in 2009 68 kg ha^{-1} in 2010	100 kg ha^{-1} in 2009 100 kg ha^{-1} in 2010

vices, 2012) and Em50 Data Loggers (Decogon Devices, 2012) from May 2010 to May 2011. Daily soil matric potential was recorded at the same depths and period of time using EQ2 Sensors (AT Delta-T Devices, 2012) and DL2e Data Loggers (AT Delta-T Devices, 2012). Monthly soil samples were collected from the depths of 0-30, 30-45 and 45-60 cm from May 2010 to March 2011. Soil nitrate was extracted from the soil samples with 2M KCl using a 1:5 soil to extractant ratio. The sampling procedure was systematic; that is, at each sampling time, 10 random soil cores were bulked and one composite sample was collected for the sampling increments 0-30 and 30-45 cm. For the sampling increment of 45-60 cm, only 6 random cores were prepared due to the soil stiffness.

In-situ soil hydraulic conductivity (k_s) was measured using the Guelph Permeameter (GP) (Reynolds and Elrick, 1985) at 15 locations across the 15-ha conventional farm including the monitored location site (i.e., the sensors location). Due to soil stiffness, boreholes could not be developed to the third soil layer, and hence GP test was not performed for this layer. According to the detailed soil survey

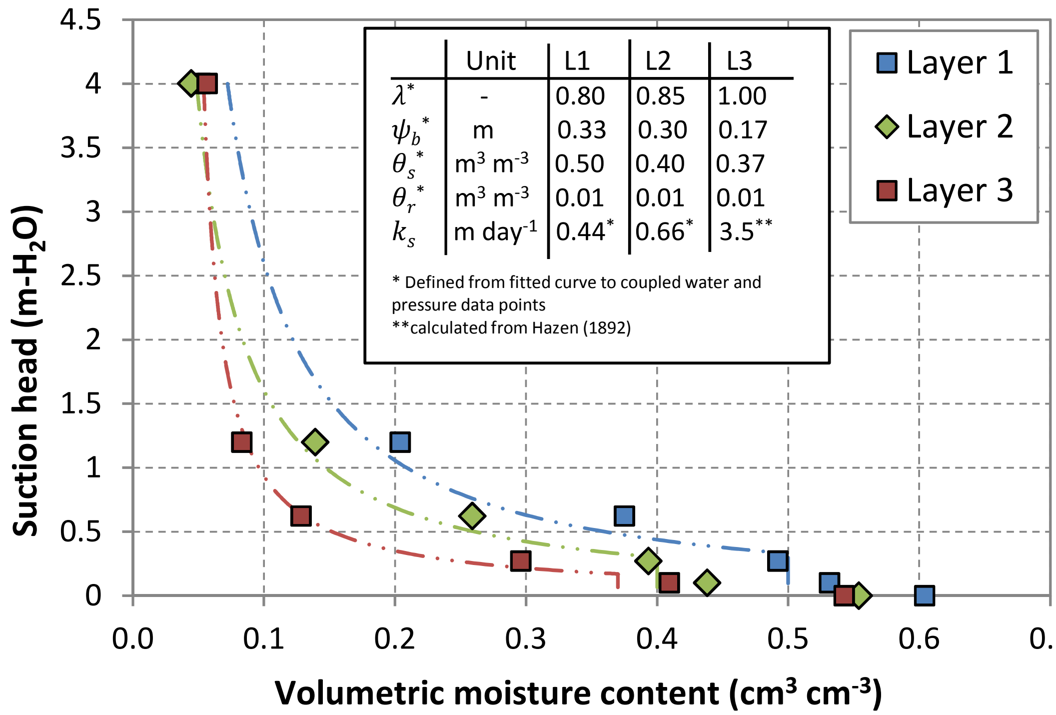

Figure 4.2: Soil moisture retention curve (SMRC). The dashed lines were fitted by adjusting λ, ψ, θ_s and θ_r. L1 to L3 represent soil Layers 1 to 3.

conducted in the location of the experiment and the boreholes prepared for the GP tests across the farm, it was discovered that the top 75 cm of the soil profile is comprised of three main soil layers: the uppermost is the agricultural soil layer, and its thickness ranges from 20 to 55 cm; the second soil layer contains less organic matter, compared to the top soil layer with lighter colour. And finally the sand soil layer which contains considerable amount of gravel and known to be the top of the aquifer. The raspberry root zone was mostly concentrated in the two uppermost soil layers.

4.2.2.1 Water flux estimation

Vertical water fluxes including up or downward capillary fluxes and downward gravity drainage were estimated from Darcy-Buckingham equation (Mallants et al., 2011):

$$q_z = -k_z(\psi)\left(\frac{\partial \psi}{\partial z} + 1\right) \tag{4.1}$$

where q_z is vertical water flux between two soil layers (m day^{-1}), ψ is soil matric potential between two layers (m), k_z is unsaturated hydraulic conductivity (m day^{-1}) at ψ, and z is the vertical distance (m). In Eq.(4.1), it is assumed that no source or sink term affects water flow between two soil layers. To meet this condition, this equation was solved between the two lowest soil layers of the monitored location site (i.e., the depth of 52 cm in the second soil layer and 70 cm in the third soil layer) using the recorded daily soil pressure data. At this vertical distance, minimum plant water uptake is expected as higher root densities are expected near the soil surface (Christensen, 1947; Bristow and Brun, 1987). The unsaturated hydraulic conductivity (k_z) between the depths of 52 and 70 cm was estimated from the Brooks and Corey (1964) relationship:

$$k_z(\psi) = \begin{cases} k_s & : if \ \ \psi \leq \psi_b \\ k_s\left(\frac{\psi_b}{\psi}\right)^{2+3\lambda} & : if \ \ \psi > \psi_b \end{cases} \tag{4.2}$$

where λ is grain size distribution index and ψ_b is air-entry water suction (m), averaged for Soil Layers 2 and 3 (Figure 4.2). The saturated hydraulic conductivity (k_s) was determined from GP test for the second soil layer. Due to lack of GP data for the third soil layer, the Hazen (1892) empirical formula was used for this soil layer to calculate saturated hydraulic conductivity based on soil particle size distribution. In Eq.(4.2), the representative k_s for the perpendicular flow from the depth of 52 cm in Soil Layer 2 to the depth of 70 cm in Soil Layer 3 was estimated from the harmonic mean (Oosterbaan and Nijland, 1994):

$$\frac{D_t}{k} = \sum_{i=1}^{n} \frac{D_i}{k_i} \tag{4.3}$$

where k represents the saturated hydraulic conductivity of the layered soil, i is the number of soil layers (i.e., two soil layers), D_t is the total thickness of the soil layers (i.e., 18 cm), and k_i is the saturated hydraulic conductivity measured for Layers 2 and 3. Due to the high amount of sand, it was assumed that macropore flow was negligible and matrix flow dominated.

4.2.2.2 Nitrate flux estimation

Nitrate is highly soluble and readily transported with water flow through the soil. Vertical nitrate flux (mg m^{-2}day^{-1}) between two soil layers was estimated from:

$$q_{NO_3} = q_z \frac{C_{NO_3}}{\theta \Delta z} \tag{4.4}$$

where q_z is the vertical water flux (m day^{-1}), C_{NO_3} is the average bulk soil nitrate concentration (mg m^{-2}day^{-1}) and θ is the average volumetric soil water content (m^{3}m^{-3}) in Δz soil thickness (m). Similar to water flux estimation, vertical nitrate flux was calculated between the depths of 52 cm in the second soil layer and 70 cm in the third soil layer.

Soil nitrate concentration (C_{NO_3}) was measured on approximately a monthly basis starting May 2010 and ending March 2011, totalling nine measurement events. Due to the lack of daily measurements, unlike water flux, nitrate flux could be calculated only for the nine events. Therefore, the performance of the model to simulate nitrate flux was evaluated on those dates by calculating model estimation error. That is, maximum error of simulated q_{NO_3} was propagated based on the errors in different quantities of Eq.(4.4); meaning the summation of the simulation error (absolute error in the measurement divided by the size of the measurement) in q_z, C_{NO_3} and θ. Because C_{NO_3} was not measured for the depths below 45 cm, the average estimation error for the depths of 0-15, 15-30 and 30-45 cm was adopted as the estimation error of the depths below 45 cm.

4.2.3 Modeling

4.2.3.1 CoupModel description

The one-dimensinal CoupModel or Coupled Model (Jansson and Karlberg, 2012), formerly known as SOIL or SOILN-models (Eckersten et al., 1998), simulates coupled fluxes of heat and water in a layered soil profile. In the CoupModel, nitrogen and carbon turnover, and plant development are also simulated. The soil water retention function is expressed with either the Brooks and Corey (1964) or van Genuchten (1980) function, and the soil water movement is simulated using Richards' equation. Soil macropores are accounted in the model with an implicit relationship that partitions infiltration into ordinary Darcy flow and bypass flow. Snow, intercepted water and surface ponding are accounted at the upper soil boundary. Nitrogen enters into the soil system from above (as plant litter, dry/wet deposition and fertilizer) and below the ground surface (SOM decomposition). SOM is partitioned into the humus pool, litter pool, surface litter pool and faeces pool (if manure is applied). When litter falls, it first enters the microbial-inactive surface litter pool. Then, it gradually enters the litter and humus pools. Various options/approaches are available in the CoupModel for simulating plant growth or biomass production (leaf assimilation). Assimilated carbon then allocates to different parts of the plant: root, leaf, stem and grain. The carbon content in different parts of the plant gives rise to nitrogen uptake and allocation in accordance with the parameterized C:N ratio. Inorganic-N dynamics are simulated based on the nitrogen cycle, soil mineral nitrogen concentration and soil water flow in different soil layers. A more detailed description of the model is given by Jansson and Karlberg (2012).

4.2.3.2 Model application

The modeling approach and settings in this study are similar to those used for the calibrating site; only farming practices of the calibrating site were replaced with those of the conventional farm (Table 4.2). Meteorological data including daily precipitation, wind speed, average temperature and relative humidity were obtained from the Abbotsford Airport weather station database (Environment Canada, 2012a). Average cloudiness parameter (65%) was taken from Natural Resources Canada (2012). The CoupModel uses this parameter to estimate radiation. The Brooks and Corey (1964) function was selected to express the water retention function and the unsaturated hydraulic conductivity. Unit gradient flow was assumed as the lower boundary condition. Microbes were represented implicitly; that is, decomposition of organic matter (litter and humus pools) is substrate controlled, and follows the first-order rate law. Decomposition rate is governed by the response functions of soil temperature and soil moisture. A common soil temperature response function (Ratkowsky et al., 1982) and a standard soil moisture response function were used (Jansson and Karlberg, 2012). Atmospheric nitrogen deposition was accounted for in the simulation by two parameters: dry deposition of nitrogen (0.001 g N m^{-2} per day) and concentration of nitrogen minerals in precipitation (0.34 mg N L^{-1}) (Environment Canada, 1997). The Penman-Monteith equation (Monteith, 1965) was used to simulate ET. Plant water uptake parameters were set to their default values. The canopy resistance in the Penman-Monteith equation is proportional to the maximum leaf conductance of fully open stomata (g_{max}) and leaf area index (A_l). Leaf area index was set to 4 (Scurlock et al., 2001). The water use efficiency approach was adopted for simulating raspberry growth. In this method, the actual transpiration is the driving force of the carbon assimilation by plant:

$$C_{Atm \to a} = \varepsilon_w . \eta . T_a \tag{4.5}$$

where ε_w is the water use efficiency coefficient, η is the conversion factor for biomass to carbon, and T_a is the actual transpiration. Proportioned to the C:N ratio of the plant, carbon assimilation acts as a driving force for nitrogen uptake from the soil.

In this study, water and nitrate fluxes were simulated for the conventional raspberry farm, using three sets of parameters:

The transported model. This is the exact calibrated and validated model obtained for the growers' common practice treatment at the calibrating site. This model includes a total of five calibrated hydraulic parameters for three soil layers and six calibrated SOM and growth parameters (Table 4.3). Based on the information obtained from the soil map of the Lower Fraser Valley and the detailed soil surveys conducted for the calibrating site and the conventional raspberry farm, it was inferred that the uppermost 1 m soil profile consists of three soil layers with similar characteristics in corresponding layers; accordingly, it was assumed that properties of the corresponding soil layers are similar. Five hydraulic parameters associated with the Brooks and Corey relationship were taken from the calibrating site for each soil layer (Table 4.3) and used for the conventional raspberry farm.

The transported soil organic parameters included the decay efficiency of litter ($f_{e,l}$) and soil humus ($f_{e,h}$) pools and rate coefficient of litter (k_l) and soil humus (k_h) pools. These parameters depend on the quality of the SOM, soil type and the environmental conditions; therefore, it was expected that by having similar weather conditions, soils and cropping history and practices, these parameters are valid at the conventional farm. The initial SOM was not defined for the conventional farm. As both the calibrating and the conventional raspberry farm had similar agricultural background , the average SOM measured at the calibrating site (that is, 0.0325 gr OM gr^{-1}soil) was used. The transported growth parameters included the maximum leaf conductance of fully open stomata (g_{max}) and the water use efficiency coefficient (ε_w). These parameters are crop dependant, and hence are constant for raspberry crop. These two parameters were calibrated simultaneously for different treatments of the calibrating site and only one value was obtained for each parameter.

The transported model with locally-measured hydraulic parameters. Soil hydraulic parameters of the transported model were replaced by the locally-measured values (Table 4.3). Soil hydraulic parameters at both sites were measured with the same spatial density (i.e., at one location) and laboratory analysis techniques (see

Table 4.3: Hydraulic, organic matter and crop parameters used.

Parameter		Soil layer	Unit	Transported	Locally measured	Up-scaled
Soil hydraulic parameters	Pore size distribution index (λ)	L1 L2 L3	-	0.36 0.38 0.53	0.8 0.85 1	0.79 0.88 -
	Air-entry water suction (ψ_b)	L1 L2 L3	m	0.30 0.26 0.07	0.33 0.30 0.17	0.55 0.20 -
	Saturation water content (θ_s)	L1 L2 L3	m^3m^{-3}	0.50 0.40 0.44	0.50 0.40 0.37	0.50 0.40 -
	Residual water content (θ_r)	L1 L2 L3	m^3m^{-3}	0.04 0.03 0.03	0.01 0.01 0.01	0.01 0.01 -
	Saturated hydraulic conductivity (K_{sat})	L1 L2 L3	m day^{-1}	0.42 0.89 8.16	0.44 0.66 13.50	0.12 0.63 -
Organic matter parameters	Decay efficiency of litter ($f_{e,l}$)	-	day^{-1}	0.6	No Change	
	Decay efficiency of soil humus ($f_{e,h}$)	-	day^{-1}	0.5		
	Rate coefficient of litter (k_l)	-	day^{-1}	5×10^{-5}		
	Rate coefficient of soil humus (k_h)	-	day^{-1}	0.03		
Plant parameters	Maximum leaf conductance of fully open stomata (g_{max})	-	m s^{-1}	0.025		
	Water use efficiency coefficient (ε_w)	-	g C $kg^{-1}H_2O$	5.9		

Chapter 3).

The transported model with farm-scaled hydraulic parameters. Soil hydraulic parameters of the transported model were replaced by the farm-scaled parameter values (Table 4.3).

4.2.4 Integrating Soil Hydraulic Parameters to the Farm Scale

A scaling approach was employed to integrate soil hydraulic parameters to the farm scale. The scaling approach theory was initially proposed in the work of Miller and Miller (1956). Examples of applying this method are illustrated in Tillotson and Nielsen (1984). Following the work of Miller and Miller (1956), the concept of similar media to scale soil hydraulic properties and estimate water processes across soil textures has been reformulated and extended widely (e.g., Mandelbrot (1983); Kosugi and Hopmans (1998); Tuli et al. (2001)). Scaling, in its various forms, is a convenient method to investigate the effect of spatially variable hydraulic conductivities on water flow (Vereecken et al., 2007).

The scaling approach used here is based on the similar media concept. According to this concept, two soils have similar pore space structure. That is the microscopic geometry of these soils is equal after being transformed to a reference soil with microscopic characteristic lengths, γ. For similar media, the soil water potential (ψ_i) and hydraulic conductivity (k_i) of i^{th} soil can be represented in terms of the soil water potential (ψ_r) and hydraulic conductivity (k_r) of a reference soil for the same water content with:

$$\psi_i\gamma_i = \psi_r\gamma_r \tag{4.6}$$

$$\frac{k_i}{\gamma_i^2} = \frac{k_r}{\gamma_r^2} \tag{4.7}$$

where γ_i and γ_r are the microscopic characteristic lengths of the i^{th} soil and the reference soil. Then the dimensionless scaling factor (α_i) of i^{th} soil can be calculated as:

$$\alpha_i = \frac{\gamma_i}{\gamma_r} \tag{4.8}$$

Scaling factors represent soil heterogeneity. Any soil in the set of soils with similar media assumption can be chosen as the reference soil. In this study, it was assumed that similar media conditions apply across the 15-ha conventional raspberry farm. The locally-measured soil hydraulic properties at the conventional raspberry farm were adopted as the reference soil hydraulic properties. The scaling factors for 15 locations across the conventional raspberry farm for which saturated hydraulic conductivity was measured using GP were calculated for the first and second soil layers, separately.

As suggested by Warrick et al. (1977); Sharma and Luxmoore (1979); Sharma et al. (1980), the frequency distribution of the scaling factors ($\alpha_1 ... \alpha_{15}$ for each soil layer) was described using a log-normal distribution. The median of log-normal distribution , as suggested by Sharma and Luxmoore (1979), was used to upscale locally-measured saturated hydraulic conductivity, soil water potential and finally soil moisture retention parameters. With scaled parameters, water flux from the entire conventional raspberry farm was simulated.

4.3 Results and Discussion

In the results discussed here, first, the applicability of the transported CoupModel to simulate water and nitrate fluxes at the conventional raspberry farm is quantitatively described. Also, the predictive ability of the transported model if the transported hydraulic parameters are replaced with the locally-measured parameter values was compared. Second, the replaceability of the scaled hydraulic parameters, with the measured and transported values for simulating water and nitrate fluxes from the entire conventional farm was discussed for a long-term simulation survey.

4.3.1 Applicability of the Transported Model

Total water flux estimated by the CoupModel, using the transported and locally-measured hydraulic parameters was similar (i.e., 166.4 and 167.5 cm, respectively) for the period from May 2010 to May 2011. For this period of time, water flux below the root zone was calculated as 134.4 cm using Eq.(4.1). This means that the transported CoupModel simulated water flux with error (i.e., 24% overestimation); however, application of locally-measured hydraulic parameters did not reduce this error , suggesting that the error associated with the annual water flux, simulated by the transported model, was not originated from the variability of soil hydraulic parameters between two sites. Overall, the transported model followed the seasonal fluctuations in water flow; however, simulations with local hydraulic parameters provided significantly better fit to data (R^2=87%) compared to the transported CoupModel (R^2=41%) (Figure 4.3).

The maximum nitrate flux estimation error was calculated from Eq.(4.4) by adding the errors associated with soil water content, nitrate concentration and water flux simulations. Average bulk soil nitrate concentration, measured for the depths of 0-15, 15-30 and 30-45 cm were compared to the bulk nitrate concentration, simulated for the depth of 0-45 cm using transported and locally-measured hydraulic parameters (Figure 4.4). The average soil nitrate estimation error for the nine sampling events, from May 2010 to March 2011, were 39% for the transported CoupModel and 49% for the CoupModel using local hydraulic parameters. Soil water contents simulated for the depths of 52 and 70 cm were compared to the measured values for nine measurement events (Figure 4.5). The Coupmodel constantly underestimated soil water content when local hydraulic parameters were implemented. In contrast, the transported model overestimated water content for all measurement events. The average error for soil water content estimated at

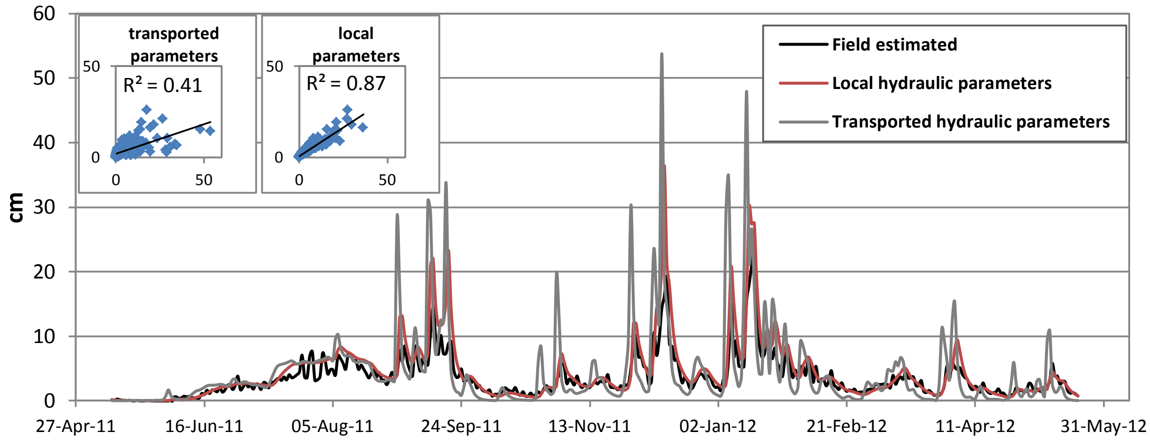

Figure 4.3: Simulated and field-estimated water flux from May 2010 to May 2012. Water flux was simulated using the CoupModel with two sets of hydraulic parameters: transported from the calibrating site and locally-measured for the conventional raspberry field.

the depths of 52 and 70 cm, using the transported hydraulic parameters (43%) was double the average error of the CoupModel simulations when local hydraulic parameters were implemented (21%). For water flux, the average error in the CoupModel estimates, using local hydraulic parameters was lower (17%, respectively) than the transported CoupModel (22%, respectively). Among soil nitrate concentration, water content and water flux, estimation error associated with soil nitrate concentration was the greatest; that is, 44%, on average, for both simulation efforts. This means, overall, soil bulk nitrate concentration estimation error is responsible for most of nitrate flux estimation error in Eq.(4.4) (Figure 4.6). Also, the difference between the performances of the two simulation efforts in predicting nitrate flux mostly originated from the difference between their soil water content estimation errors (22%). This means that the variability in soil hydraulic parameters affected soil water content more than soil nitrate concentration and water flux estimations.

The average nitrate flux estimation errors calculated from Eq.(4.4) for nine dates during May 2010 to March 2011 was 104 and 87%, using the transported and locally-measured hydraulic parameters, respectively (Figure 4.6); that is, both

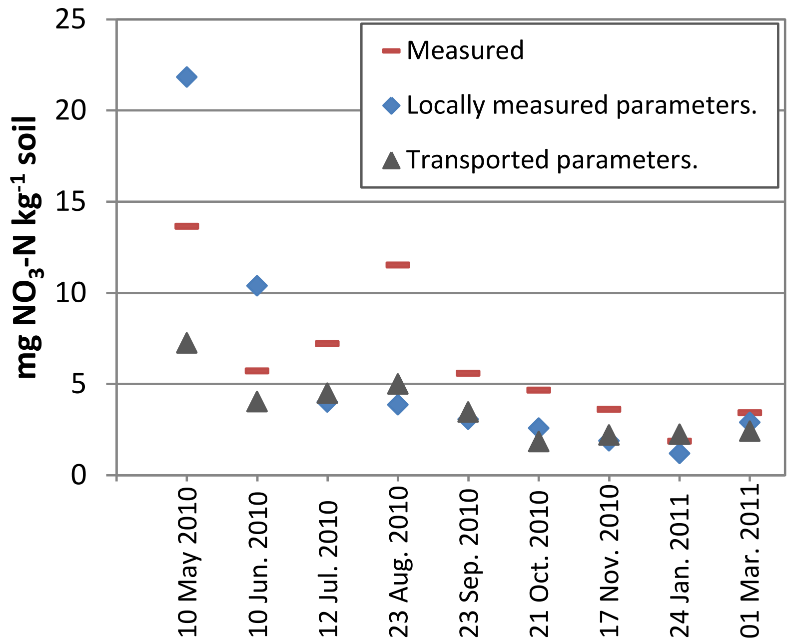

Figure 4.4: Averaged soil nitrate concentration measured for the depths of 0-15, 15-30 and 30-45 cm compared to the CoupModel estimates for the depth of 0-45 cm using the transported and locally-measured parameters.

models simulated nitrate flux with error, and using locally measured hydraulic parameters reduced simulation error only by 17% compared to the transported hydraulic parameters.

Average estimation error for September and October in which the risk of nitrate leaching is likely high due to early fall precipitation and high residual soil nitrate concentration, was 122 and 93%, using transported and locally-measured hydraulic parameters, respectively. These rates are above the average nitrate flux estimation error calculated for all measurement events for both modeling efforts. Also, the average simulation error during the growing season months including May to August (i.e., 108 and 104% using transported and locally-measured hydraulic parameters, respectively) was higher than the average nitrate flux estimation error calculated for all measurement events. The average simulation errors for late fall to early

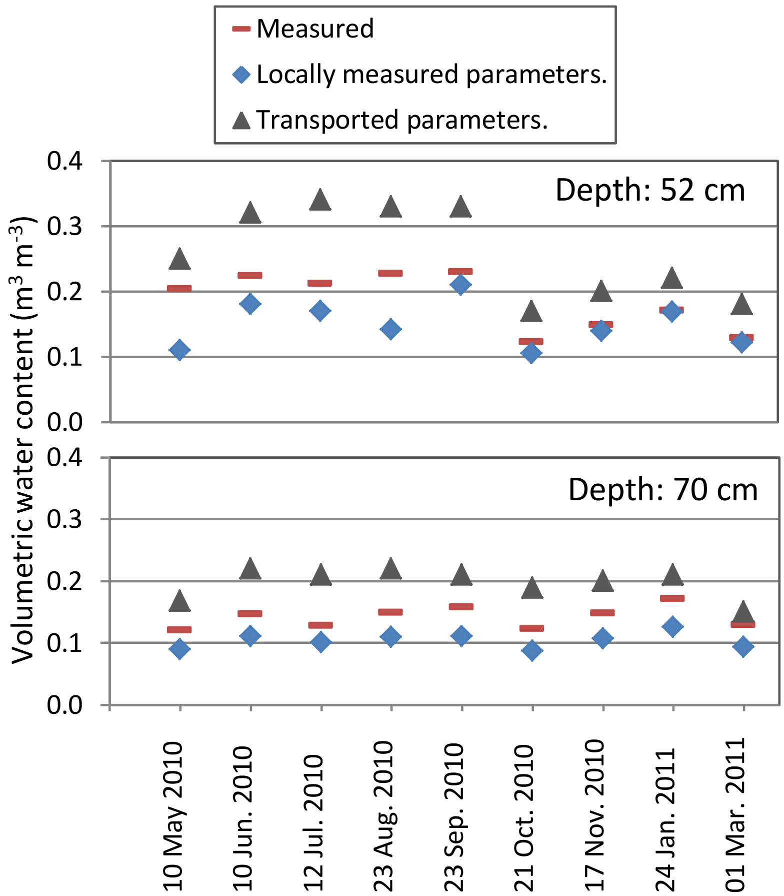

Figure 4.5: Measured and simulated volumetric soil moisture content using the transported and locally-measured hydraulic parameters for the depths of 52 and 70 cm.

spring months (i.e., November, January and March) were lower than the average nitrate flux estimation error calculated for all measurement events, using both the transported (70%) and locally measured hydraulic parameters (63%). On the basis of these findings, nitrate flux simulations are more credible for late fall to early spring than for the growing season and early fall.

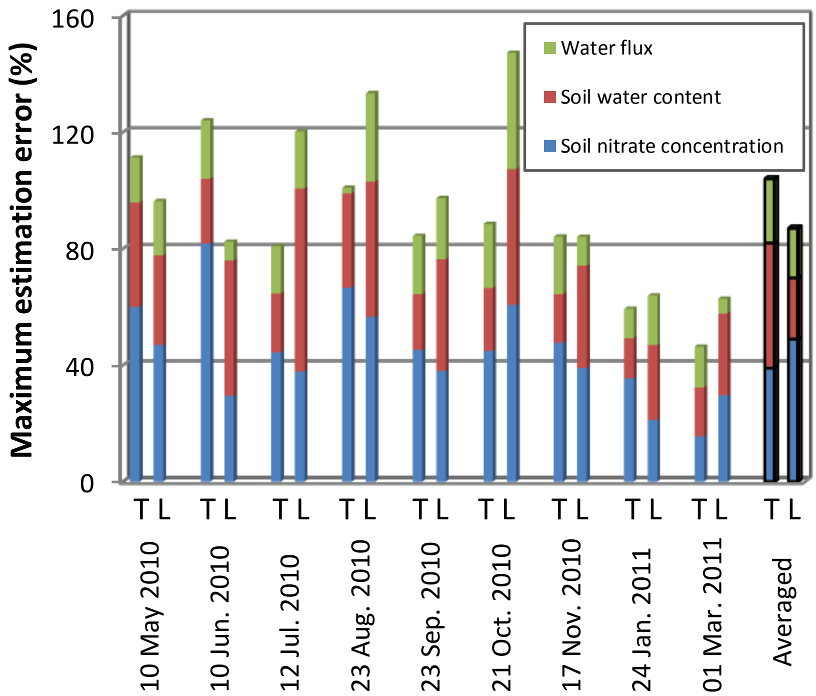

Figure 4.6: Maximum nitrate flux simulation error calculated from the sum of error associated with the simulation of soil nitrate concentration, water content and water flux for nine dates during May 2010 to March 2011, using transported (T) and locally-measured (L) hydraulic parameters.

4.3.2 Replaceability of the Conventional Farm Soil Hydraulic Parameters

Water and nitrate fluxes simulation results were integrated over the 15-ha raspberry farm. To do so, locally-measured soil hydraulic parameters were scaled to the farm level using single value scaling factor method, and resulting parameters were used for CoupModel simulation. It was assumed that the vegetative characterization and farming practices are uniform and only soil characteristics varied spatially. The scaling factor (α) for 14 locations across the raspberry farm for which saturated hydraulic conductivity was measured using GP method, were determined by using Eq.(4.7) and Eq.(4.8). The mean and standard deviation of k_s were 0.45 and 0.27

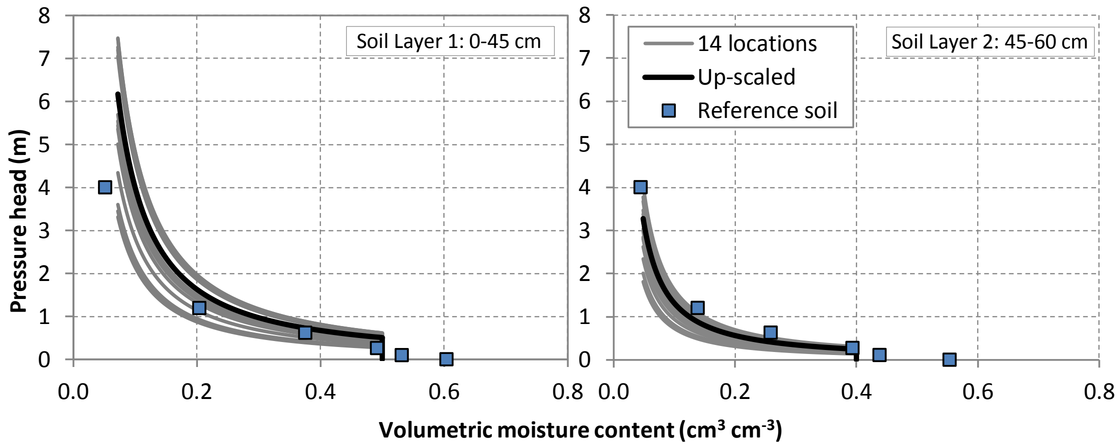

Figure 4.7: SMRC of Soil Layers 1 and 2, estimated for 14 locations within the conventional farm and up-scaled for the entire farm, using the scaling factor method and the SMRC of the reference soil.

m day^{-1} for Soil Layer 1, and 0.9 and 0.65 m day^{-1} for Soil Layer 2. The mean and standard deviation of α was calculated as 0.78 and 0.24 for Soil Layer 1 and 1.40 and 0.42 for Soil Layer 2, respectively. The higher α for the second soil layer indicates higher soil distribution index, and as a result, the presence of more sand and gravel in this soil layer which is consistent with its texture (Table 4.1). Log-normal distribution of α was generated using the mean and standard deviation of α. The median of the log-normally distributed α (0.65 and 1.22 for the first and the second soil layers) was used in Eq.(4.6) and Eq.(4.8) to integrate the SMRC of the reference soil, measured from the laboratory investigation, to the farm scale (Figure 4.7). Four Brooks and Corey function parameters including λ, ψ_b, θ_s and θ_r were modified manually to fit the farm-scaled SMRC of the first and the second soil layers (Table 4.1). Using scaled soil moisture retention and saturated hydraulic conductivity parameters, the integrated water and nitrate fluxes were simulated for 2007 to 2010. Because no data were available to scale up the soil characteristics of the third soil layer, measured parameter values for this soil layer were employed for this simulation.

Annual water flux was simulated for 2007 to 2010, using transported, locally-

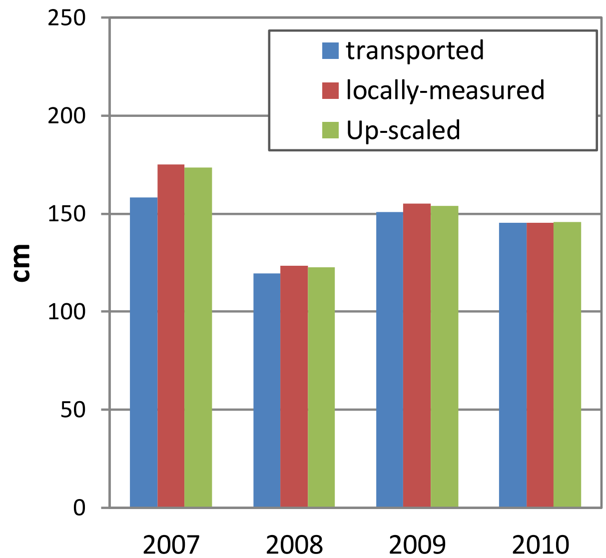

Figure 4.8: Annual water flux estimated by the CoupModel using transported, locally-measured and up-scaled hydraulic parameters.

measured and scaled soil hydraulic parameters (Figure 4.8). The effect of soil variability in the conventional raspberry farm on water flux was negligible; that is, estimated annual water flux using the locally-measured hydraulic parameters (i.e., the reference soil) and the scaled hydraulic parameters were similar during the four-year survey. Except for the first year of the survey (i.e., 2007) in which annual water flux, simulated by the transported model was 10% less than the simulation result obtained from the locally-measured and scaled hydraulic parameters, the annual water flux simulations using all three parameter sets were similar. This long-term investigation suggested that, in general, water flux simulation using the three sets of hydraulic parameters were comparable, and that in the absence of local parameter values, transported values can be used to simulate water flux in the farm scale.

For 2007, annual nitrate leaching was simulated as 266, 340 and 297 kg ha^{-1} using the transported, locally-measure and integrated hydraulic parameters, respectively. That is, the annual nitrate leaching simulated by the local hydraulic parameters was 28 and 20% higher than the estimates using the transported and scaled parameters, respectively. Also, integrated nitrate leaching for 2007 was 12%

more than the transported model estimates. However, for the subsequent years, the differences between nitrate flux simulations were negligible (Figure 4.9). In 2007, a significant amount of 744 kg N ha^{-1} was applied as poultry broiler litter. According to British Columbia Ministry of Agriculture and Lands (2009), 33% of total nitrogen is available in the year of application. This means that mineralization of manure is a significant contributor to nitrate leaching. Therefore, the considerable differences between nitrate leaching estimated in 2007 suggests that simulation of manure mineralization is sensitive to the variability of soil hydraulic properties, and that the transported hydraulic parameters cannot substitute the locally-measured hydraulic parameters for simulating nitrate leaching in the conventional raspberry farm in 2007. Also, the integrated hydraulic parameters cannot be replaced by the transported values for representing spatial variability across the farm. According to the CoupModel simulation (Figure 4.9), the annual nitrate leaching for 2008 (i.e., average 101 kg ha^{-1} for all three modeling efforts) is considerable suggesting that the mineralization of manure continues in 2008, supplying a significant amount of mineral nitrogen to the soil. However, in contrast to 2007, nitrate leaching estimations, using transported and locally-measured and scaled hydraulic parameters were similar. This infers that the variability of soil hydraulic properties influenced nitrate leaching only in the same year of manure application; that is, when the organic matter is fresh and labile.

For 2007 to 2010, simulated nitrogen uptake using transported, locally-measured and scaled hydraulic parameter was similar, with slightly higher rates for the local hydraulic parameters. It was concluded that all parameter sets had similar effect on plant nitrogen uptake, and soil variability across the field had no effect on plant nitrogen uptake. Hence, locally-measured and scaled parameters are replaceable with the transported values for simulating nitrogen uptake in the conventional farm. The highest plant nitrogen uptake was simulated for 2007 (i.e., 140 and 136 kg ha^{-1} for the transported and locally-measured hydraulic parameters) possibly due to the abundant nitrogen supply and faster growth rate in the first year of plant establishment. The lowest plant nitrogen uptake was simulated for 2008 (i.e.,

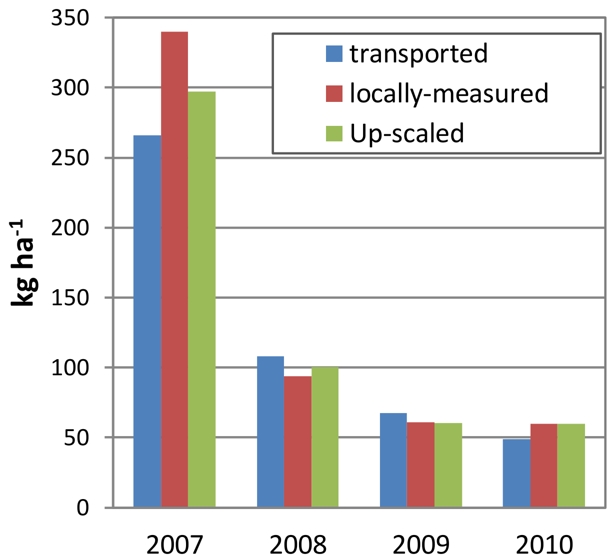

Figure 4.9: Annual $NO_3^- - N$ leaching estimated by the CoupModel using transported, measured and up-scaled hydraulic parameters.

107 and 100 kg ha^{-1} for the transported and locally-measured hydraulic parameters) possibly because no fertilizer was applied in 2008, and mineralizable nitrogen was considerably less than 2007. Estimated plant nitrogen uptake for 2009 (119 and 111 kg ha^{-1} for the transported and locally-measured hydraulic parameters, respectively) and 2010 (131 and 123 kg ha^{-1} for the transported and locally-measured hydraulic parameters, respectively) in which synthetic fertilizer was applied were in agreement with plant nitrogen uptake estimated at the conventional treatment of the calibrating site (120 and 126 kg ha^{-1} in 2009 and 2010).

4.4 Conclusion

The purpose of this study was to investigate the capability of the calibrated and successfully validated agricultural model, CoupModel, for simulating water and nitrate fluxes below the raspberry root zone in a different location than the calibrating site within the Abbotsford region.

Using the transported model, water flux was overestimated by 24% for the period of May 2009 to May 2010; however, application of the locally-measured hydraulic parameters did not reduce this error. As a result, the transported hydraulic parameters could replace the locally-measured values for simulating seasonal water flux for this period of time. On average, nitrate flux was simulated with 104% error using the transported model. Application of the locally-measured hydraulic parameters reduced this error only by 17%. The discrepancies between simulated and field-measured water and nitrate fluxes may suggest that the assumptions made for the commercial farm management practices and used as the model input data were associated with errors. Due to the lack of continuous daily field data, nitrate flux estimation error was investigated for only one day per month through a nine-month investigation. These limited data may not reflect the capability of the model for simulating nitrate flux over time, and hence more investigation is required.

CoupModel is a one-dimensional model and simulates processes for a unit of area with single crop pattern. Therefore, combined simulation of the raspberry crop on rows and cover crop on inter-rows is not feasible. Accordingly, the influence of the management of the raspberry inter-rows on nitrate and water flux was not accounted in this study. However, spring cereals, planted in the alleys following harvest, can take up as much as 75 kg N ha^{-1} (Jeffries et al., 2005), and hence influence nitrate flux below the root zone. This can be one plausible explanation for the discrepancies between simulated and field-measured water and nitrate fluxes.

By adopting the concept of similar media and using single value scaling factor method, soil hydraulic parameters were scaled to the farm level. Using the scaled parameters, annual water and nitrate fluxes were simulated for a period of four years consisting of various types and amounts of organic and synthetic fertilizer application and climate conditions. The variability of soil hydraulic parameters across the farm had a small effect on annual water flux simulation, and hence transported parameters can be used as a substitute for the measured and scaled parameters for predicting water flux across this landscape. It was found that the variability of soil hydraulic parameters influence nitrate flux by up to 28% for the year in which manure is applied to the farm, suggesting that the simulation of organic matter mineralization is sensitive to the variability of soil hydraulic parameters. Therefore, transported hydraulic parameters cannot be used as a substitute for the locally-measured and scaled parameter values for the condition when organic matter applied to the soil is fresh and liable. The transported model's lack of success to simulate nitrate flux when manure is applied might be related to the agricultural condition to which the transported model was calibrated. That is, the calibrating site was free of manure, and as a result the effect of manure on the agricultural system was not incorporated into the calibrated parameters.

Overall, the transported model was found as applicable as the local model to the conventional farm for simulating seasonal water flow and nitrate flux (except for the year in which manure was applied). The transportability of the model could be the result of the particular characteristics of the studied landscape; that is sandy texture of the soil profile and high precipitation rate might have dominated the water and solute transport and facilitated the usability of the transported model regardless of the spatial variation of the soil hydraulic properties. However, further sampling, modeling, and validation at additional field sites with different management practices are required to properly confirm CoupModel transportability within the Abbotsford physiographic region.

The transported model can be considered as a useful tool for preliminary analysis of water and nitrate fluxes from the raspberry root zone for regional scale; but for further local analysis across the Abbotsford landscape, model parameters must be redefined from a sound scientific footing. The concept of model transportability and the approach used to investigate it is applicable for other physiographical regions in which some levels of similarity exist between different parcels within the region. A transported model is useful to investigate overall environmental impact of nitrogen that aids regional farm management studies and policy option analysis.

Chapter 5

Application of advanced nitrogen fate and transport models in evaluating beneficial management practices in agricultural landscapes

Outline

Faced with increasing nitrate concentration in the Woodstock municipal supply wells, mandatory agricultural best management practices (BMPs) were implemented in a farmland, located within the wells' capture zone in 2003 to reduce nitrate leaching. In this study, the utility of the agricultural system model: Root Zone Water Quality Model (RZWQM) to predict groundwater recharge and nitrate leaching, and the long-term reduction of nitrate load to the groundwater as a result of BMP implementation were investigated at different locations within the wells' capture zone. Using field-measured soil moisture content and nitrate concentration, selected input parameters were calibrated and validated. Except for the top-soil, simulated soil nitrate content was in agreement with the field measurements for all investigated locations, with RMSE ranging from 0.6 to 9.0 mg $NO_3^- - N$ kg^{-1} soil. Simulated groundwater recharge and nitrate leaching, using the calibrated model were out of field estimated bounds; however, due to the errors and uncertainties associated with the measurement techniques and calculation assumptions, it was not possible to evaluate the actual performance of the model. The long-term effect of BMP on nitrate leaching was different at various locations, ranging from 54% reduction to 9% increase during a nine-year period. Post BMP nitrate leaching was simulated as not necessarily being less than before BMP activation. This finding conformed the field observations and infers that BMP effectiveness needs to be investigated over a long period of time and single field measurements cannot address the impact of BMP on nitrate leaching. No relationship was found between soil nitrate concentration and nitrate leaching, suggesting that soil nitrate concentration cannot be used as BMP effectiveness index. At the end of this study, the anticipated effects of two alternative BMP scenarios on nitrate leaching from a farmland under conventional agricultural practice were simulated.

5.1 Introduction

Groundwater nitrate contamination associated with the application of organic and synthetic nitrogen fertilizers on agricultural lands has led to the adoption of beneficial management practices (BMPs). BMPs are farming methods that optimize economic, environmental and agronomic efficiency in production agriculture. These practices may include choosing the most suitable nitrogen source, timing nitrogen application when it is most required by the crop, managing water flow by selecting an appropriate irrigation system and schedule, applying nitrogen based on realistic yield expectations, using soil report card to define required nitrogen supply, or using crop rotation and cover crops during non-growing seasons to minimize loss of excess nitrogen (Lilly, 1997). An essential element of BMP application includes evaluating its effectiveness. The environmental effectiveness of BMPs has been determined not only from field monitoring, but also by means of modeling. Considerable difficulties are associated with monitoring approaches and measurement techniques used to evaluate BMPs effectiveness. For example, a substantial lag time often exists between the time when the BMP is employed and the associated groundwater quality responses due to the complexity of the interconnection between the soil surface and groundwater (Tomer and Burkart, 2003; Shukla, 2000). Moreover, BMP effectiveness is site-specific, and hence monitoring results cannot be adopted at ungagged locations with different climate, hydrologic settings, geologic environments and agricultural land uses (Dillaha, 1990). Models are cost-effective tools not only to interpret field-measured data but also to evaluate BMP effects prior to its implementation. Since monitoring programs require a long period of data collection, many BMP evaluation studies have been based on modeling analysis. Stone et al. (1998) utilized the Gleams model for simulating the reduction in groundwater nitrate concentration as a result of BMP implementation on a swine waste spray field (Coastal Bermuda grass) located in the Cape Fear River Basin of North Carolina during a five-year study. According to Stone et al. (1998), modeling results were consistent with the field observations. Morari et al. (2004) investigated the effects of alternative BMPs in the Mincio River Basin in northeastern Italy, using a GIS integrated CropSyst model. They demonstrated that efficient irrigation is the key factor for nutrient management to minimize nitrate leaching, and to promote sustainable agricultural development, and that the integrated model is a useful tool to support BMP decisions. Using the process-based water and nitrogen management model (WNMM), Hu et al. (2010) concluded that nitrate leaching was significantly reduced under the existing management practices suggested by farm extension personnel; however, the water and nitrate inputs still far exceeded the crop demand under desert oasis conditions in northwestern China.

Hydrogeological studies at the Thornton Well Field, located in Woodstock On-

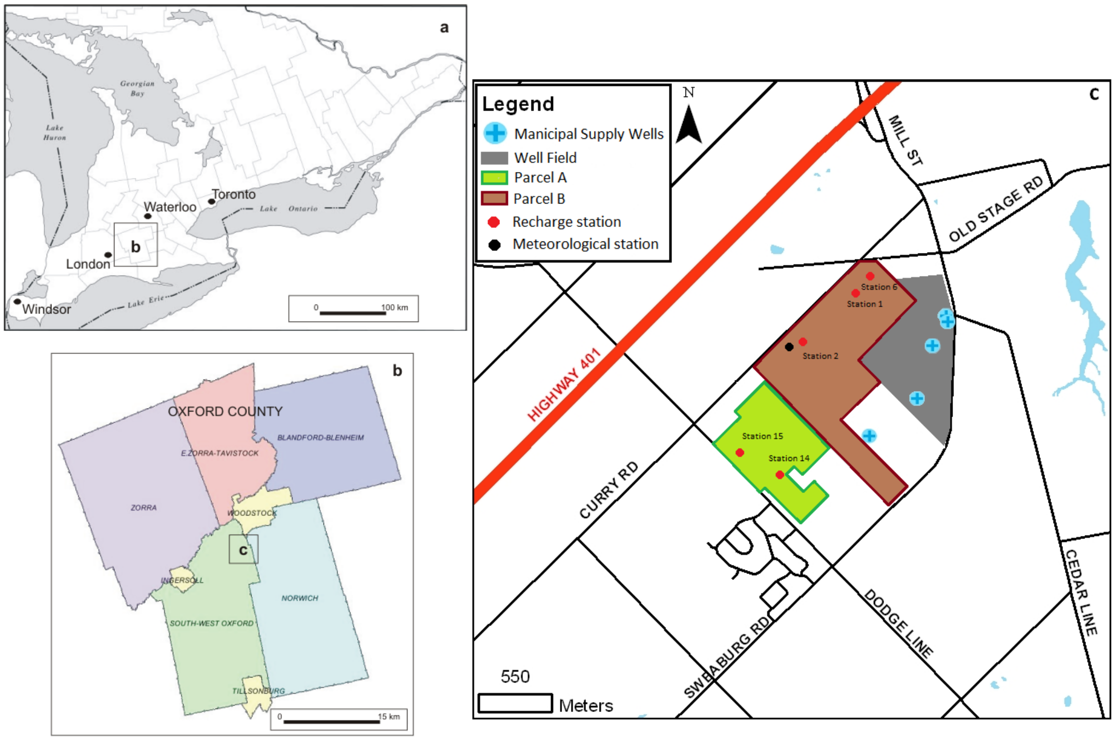

Figure 5.1: a) Location of Oxford County within Southern Ontario. b) Location of study site within Oxford County. c) Farm land field number designations within Parcels A and B. (Adapted from Koch (2009)).

tario (Figure 5.1), were initiated in response to rising nitrate concentration in the municipal supply wells. The nitrate concentration of selected wells at this site exceeded the drinking water limit (MAC of 10 mg $NO_3^- - N$ L^{-1}) in the mid-1990s. The correlation between extensive fertilizer use since the 1950's and nitrate concentration increase suggests that the agricultural land use in the vicinity of the well field is the nitrate source. In an effort to reduce the nitrate concentration, the County of Oxford purchased 111 ha of the farm land including parcel A and B (Figure 5.1) in 2003 within the capture zone of the municipal supply wells. Parcel B was rented to farmers who farm it under nutrient application restrictions.

Field investigations have been conducted at the Thornton Well Field to study the effects of the BMPs on nitrate loading and the groundwater quality. Haslauer

(2005) quantified the nitrate stored in the unsaturated zone and determined the potential decrease in nitrate concentrations at the well field associated with no nitrate application on Parcel B. Bekeris (2007) estimated nitrate mass flux at eight stations within Parcel B during 2005 and 2006. Bekeris (2007) scaled up these point scale nitrate flux values to the field scale based on topography, geology and field observations and concluded that there was a beneficial response to the BMP at locations with shallow sandy stratigraphy and low nutrient requirement crops. Many of the methods such as soil coring in the vadose zone, and recharge and nitrate leaching estimation techniques developed and used by Bekeris (2007) were employed by Koch (2009) who continued to monitor and evaluate the effects of the BMP at the eight original stations plus seven new stations during 2007 and 2008. Koch (2009) concluded that the adopted BMPs were successful in reducing nitrate concentration but there was a long lag time between BMP implementation and impact on groundwater quality in deeper aquifers. Due to positive results of the nutrient management, Koch (2009) suggested to continue BMP implementation within Parcel B and initiate the practices within Parcel A.

This study investigates 1) the utility of the agricultural system model Root Zone Water Quality Model (RZWQM) (Ahuja et al., 2000c) to predict groundwater recharge and nitrate leaching, and 2) the long-term reduction of nitrogen load to the groundwater as a result of BMP implementation. RZWQM is a detailed research model (Shaffer, 2002) that features complex soil hydrological and nitrogen cycle processes for cropped systems. Selected soil hydraulic, organic matter and crop growth parameters were calibrated and validated using the field observations that were collected by Bekeris (2007) and Koch (2009) at three original stations with dominant BMP cropping practices and distinctive soil geology. The RZWQM has been used in various calibration and validation studies, but only in a few studies were automatic parameter estimation methods used (Fang et al., 2010; Nolan et al., 2010; Malone et al., 2010). In this study the heuristic optimization algorithm Dynamically Dimensioned Search (DDS) (Tolson and Shoemaker, 2007) was utilized for the calibration of RZWQM. Finally, the anticipated effects of two alternative

BMP scenarios on nitrate leaching from Parcel A were simulated.

5.2 Materials and Methods

5.2.1 Site Description

The precipitation at the study site is relatively uniform during the year totaling 950 mm on average. The mean monthly temperature ranges from $-6.3\,^{\circ}\mathrm{C}$ in January to $20.4\,^{\circ}\mathrm{C}$ in July with an annual average of $7.5\,^{\circ}\mathrm{C}$ (Environment Canada, 2012b). The hydrogeological system at this site is of glacial origin resulting in variable geometry. According to Haslauer (2005), the hydrogeological system consists of four aquifers and four aquitards overlying a bedrock aquifer. The thickness of each hydro-stratigraphic unit ranges from zero to tens of meters over the site. The extraction wells in the Woodstock Well Field are completed in Aquifer 3. The dominant soil is the Honeywood-Guelph complex composed of mixed silty alluvial deposits over loam till (Haslauer, 2005). The topography is gently rolling with a ground elevation ranging from 300 to 330 meters above sea level. The surface water drains into Cedar Creek which is a tributary of the Thames River (Haslauer, 2005).

Parcels A and B are divided into three and eight agricultural fields, respectively. In the research efforts of Bekeris (2007) and Koch (2009), groundwater recharge and nitrate mass load were assessed at various locations ("recharge stations") within these fields to represent a variety of topographic, geologic and agricultural management conditions. For this study, one field from Parcel A (Field A1) with two recharge stations (Stations 14 and 15) and two fields from Parcel B (Fields B4 and B7) with three recharge stations (Stations 1, 6 in B7; and Station 2 in B4) were selected. These agricultural fields represent the most dominant cropping practices within Parcel A and B, and each of their associated recharge stations has distinctive soil geologic characteristics. The locations and topography of the selected recharge stations are summarized in Table 5.1. The shallow composite geologic logs compiled

Table 5.1: Location and the topography of the selected recharge stations.

Recharge station	Parcel-Field	Topography
1	B-7	low-flat
2	B-4	high-flat
6	B-7	slope
14	A-1	low-slope
15	A-1	slope

from borehole logs for the selected recharge stations are presented in Figure 5.2. Stations 1 and 6 are located within the glaciofluvial outwash channel and can be characterized by sand and gravel, with some silt layers at Station 6. The water table in Aquifer 2 fluctuates from 2.2 to 3.3 m below ground surface (bgs) at Station 1, and from 8.9 to 10.0 m at Station 6. Station 2 includes a shallow stratigraphy composed of clay-silt till which is interpreted as Aquitard 1. The till is underlain by unsaturated silty sand layer. The depth to Aquifer 3 water table ranges from 26 to 26.4 mbgs at Station 2. Stations 14 and 15 are comprised mostly of loose sand associated with Aquifer 2. The water table at these stations is believed to be located approximately 22 and 30 mbgs, respectively. In general, the majority of the study site is overlain with distinctly permeable sediments (Padusenko, 2001).

Crops planted and nitrogen application for the selected fields since the purchase of Parcels A and B by the County in 2003 to 2008 are summarized in Table 5.2. The most common cultivated crops are corn, soybeans, wheat and grass. Corn is typically given starter fertilizer at planting which is followed with sidedress nitrogen in late spring. Due to the ability to fix atmospheric nitrogen, soybean is not fertilized. Historical land use and nitrogen application are not available prior to 2003. Anecdotal information from former farmers suggests that wheat-corn-soybean rotation was the common practice. Hard red winter wheat which requires high nitrogen input was planted in the rotation, but since 2003, this crop has been replaced by soft red winter wheat which requires almost 50% less nitrogen. Yearly nitrogen application rates prior to 2003 were approximated based on recommended and commonly

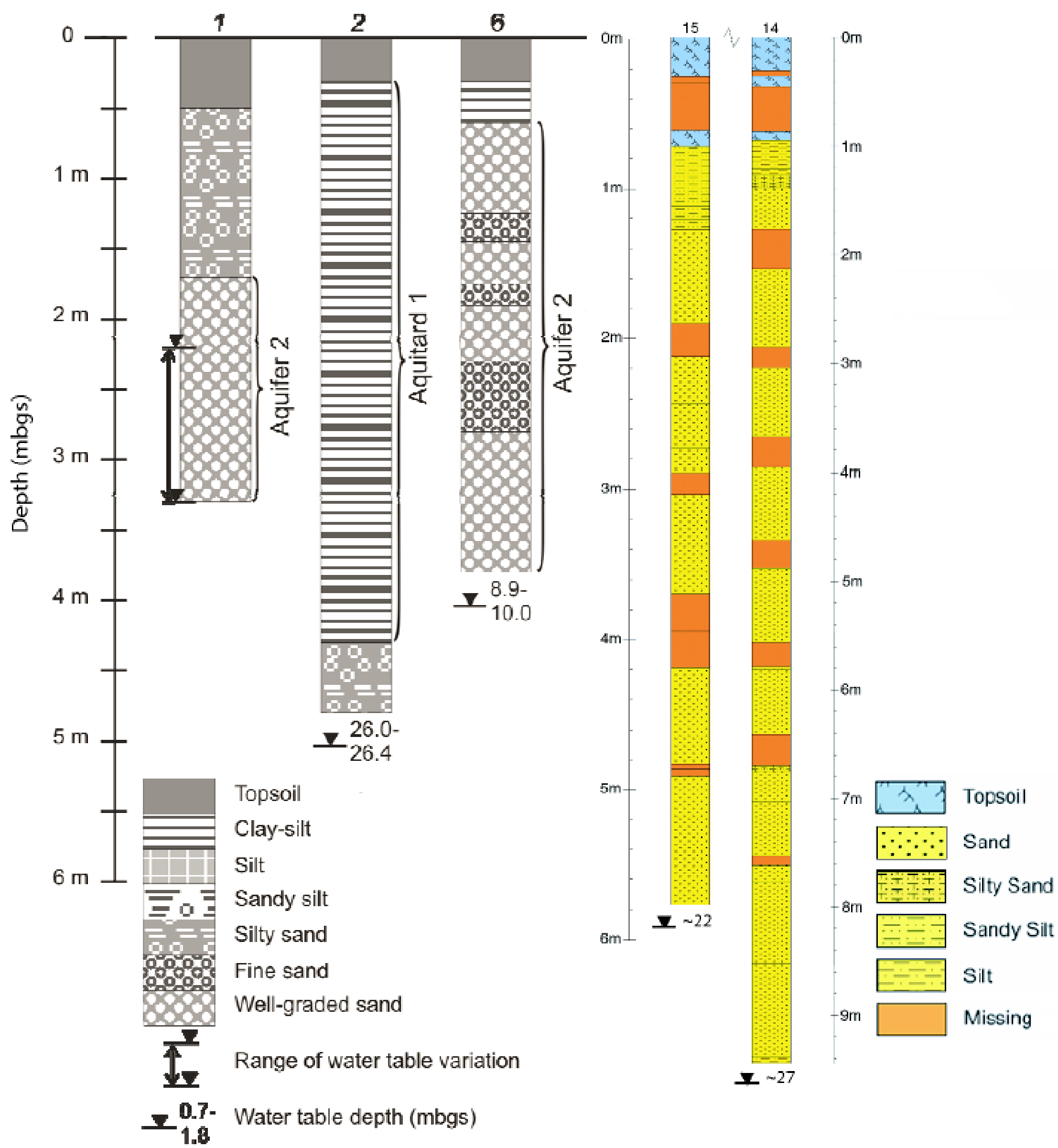

Figure 5.2: Shallow composite geologic log and water table location at selected recharge stations (Stations 1, 2 and 6 were adopted from Bekeris (2007), and Stations 14 and 15 were from Koch (2009)).

Table 5.2: Planted crops and nitrogen application rates (kg h^{-1}) history at the selected fields within the study site since BMP practice activation. n/a = data not available.

Parcel	Field	2003		2004		2005		2006		2007		2008	
A	1	Corn	78 (May) 60 (Jun.)	Corn	90 (Jun.)	Corn	91 (May) 60 (Jun.)	Corn	91 (May) n/a (Jun.)	Corn	n/a	Corn	112 (May)
B	4	Soybean W.wheat	0 6.2 (Oct.)	W.wheat red clover	65 (May)	Corn	27 (May) 62 (Jun.)	Romano beans W.wheat	26 (Jun.)	W.wheat red clover	90 (Apr.)	Corn	50 (Jun.)
	7	Soybean W.wheat	0 6.2 (Oct.)	W.wheat red clover	65 (May)	Oat/ grass	9.7 (Apr.)	Grass	0	Grass	0	Grass	0

Table 5.3: Recommended and assumed historical nitrogen application rates (estimated by Soil Resource Group (2006), adopted from Koch (2009)).

Crop	Regular nitrogen application (kg ha^{-1})	Notes
Corn	157-190 annual total	May be reduced by planting red clover with wheat in the preceding year
Hard red winter wheat	157-168 (134 minimum)	Crop's value dependent on protein content
Soft red winter wheat	100	Low protein content is desirable
Soybean	0	Nitrogen fixer

used nitrogen application rates (Table 5.3). Since 2003, nitrogen applied to corn and wheat crops within Parcel B has been reduced by 46% (Koch, 2009). Another BMP practice that has been activated to reduce nitrogen application was to plant N-fixing soybean regularly. Field 7 previously contained a livestock farm. It is likely that produced manure was applied to this field. In order to mine nitrogen from shallow and highly permeable soil in Field B7, grass and oat were planted together on this field since 2005.

5.2.2 Field Data

Groundwater recharge rates and nitrate mass flux through the unsaturated zone were measured using a tracer movement method by Bekeris (2007) and Koch (2009). Sodium bromide (NaBr), a conservative tracer, was applied at ground surface at the recharge stations within Parcel B between July 20 and 22, 2005 at a rate of 0.45 kg Br m^{-2} (Bekeris, 2007) and at all recharge stations within Parcel A and B between January 8 and 9, 2008 at a rate of 0.47 kg Br m^{-2} (Koch, 2009). Several rounds of geologic cores were collected for analysis of soil water content and nitrate concentration, and the applied bromide tracer for each recharge station. Using bromide concentration data, recharge rate was approximated in the zone of tracer migration as the product of the tracer's vertical velocity and the average volumetric water content. Nitrate mass flux was estimated by multiplying the average pore-water nitrate concentration by the recharge rate at the associated stations. Details of the instruments installed, tracer application, sampling, laboratory analyses and recharge and nitrate mass flux estimation methods are given in Bekeris (2007) and Koch (2009).

5.2.3 Model Application

5.2.3.1 Root Zone Water Quality Model

The one-dimensional Root Zone Water Quality Model (RZWQM) is an integrated physical, chemical and biological process model that simulates water and solute movement, heat flux, plant growth and nitrogen and carbon turnover as the result of soil management activities (Ahuja et al., 2000a). In the RZWQM, soil hydraulic parameters are described with the Brooks and Corey (1964) relationships while water distribution is calculated using Richards' equation. The model can account for macropore flow with a concept similar to the transient flow models of Hoogmoed and Bouma (1980), and Beven and Germann (1981). The extended Shuttleworth-Wallace model is used to simulate ET (Farahani and Ahuja, 1996).

Root water uptake is simulated using the approach of Nimah and Hanks (1973). In the RZWQM, soil organic matter (SOM) is partitioned into five computational pools based on their physical and chemical properties: fast and slow residue pools; and fast, intermediate and slow humus pools. Material in an organic matter pool can be transformed into other pools, assimilated into microbial biomass or emitted as CO_2. Decomposition of SOM is modeled as a first-order reaction. The RZWQM includes a Generic Crop Growth Model and DSSAT 4.0 Crop growth model (Tsuji et al., 1994). Also, the RZWQM is implemented with a simple module, Qckplant, which mimics plant growth by only taking water and nutrients from soil. This option is suitable when detailed growth parameters are not available or the model user is interested in simulating environmental impacts only. The Qckplant module does not simulate photosynthesis and yield, and requires modification of limited number of parameters including length of the growing season, winter dormancy recovery date, rooting depth and seasonal plant nitrogen uptake. When Qckplant module is used, seasonal nitrogen demand is partitioned into daily values. Therefore, plant N-uptake is relative to N-demand and soil N-availability. A comprehensive description of the RZWQM is provided by Ahuja et al. (2000b).

5.2.3.2 Model Application

The agricultural system at the selected recharge stations within Parcel A and B were simulated using the RZWQM over a period of 16 years, from January 1997 to December 2012. Required weather data included daily maximum and minimum air temperature, wind speed, relative humidity and precipitation data. These data were obtained from a local meteorological station installed within the study field for December 2004 to July 2008. Required weather data for other months were obtained from the Woodstock, ON Station (43.14 °N, 80.77 °W, 281.9 masl) (Environment Canada, 2012b), and missing data were filled using data from the London-Airport Station (43.03 °N, 81.15 °W, 278 masl) (Environment Canada, 2012b). Since the Environment Canada weather stations did not have shortwave radiation data, the RZWQM climate generator was used to randomly generate shortwave radiation data for the nearest weather station (i.e., Lockport, NY, USA) for the period of January 1997 to December 2004, and from July 2008 to December 2012.

The main components of the RZWQM for simulating agricultural systems include soil physical processes, nutrient dynamics and cropping management. The Brooks-Corey relationship (Brooks and Corey, 1964) was used to describe soil moisture retention properties and unsaturated hydraulic conductivity. Required parameters included saturated hydraulic conductivity (K_{sat}), saturated soil moisture content (θ_s), residual soil moisture content (θ_r), bubbling pressure head (ψ_b) and the pore size distribution index (λ). Initial estimate of some of these parameters based on laboratory analysis and literature data are provided in Bekeris (2007). However, the solution to Richards' Equation fails to converge with the combination of all initial parameter values due to the nonlinearity of the Richards' equation and the heterogeneous nature of the soil profile. Therefore, only soil particle fractions and bulk density (ρ_b) were utilized from Bekeris (2007) (Table 5.4). In the RZWQM, when soil particle fractions are modified, the closest available soil class to that particle combination and its related hydraulic parameters (Rawls et al., 1998) is used automatically from the RZWQM database. Soil bulk density defines porosity which is used as the saturated soil moisture content in the Brooks-Corey relationship. The lower boundary condition of the soil profile for Stations 2, 6, 14 and 15 was set as a unit hydraulic gradient flow. The lower boundary condition at Station 1 was set as constant flux to account for high water table. Also, the initial water content of the soil profile at run start was defined as tensiometric potential at Station 1, with the location of the initial water table defined with positive potentials. The horizontal/lateral hydraulic gradient of Aquifer 2 was set as 0.009 m m^{-1} (Bekeris, 2007) at Station 1.

The cropping history of the agricultural fields was not available prior to 2003; therefore, a cropping rotation and nitrogen application schedule, based on available information, recommended by the Soil Resource Group (2006) for nitrogen application rates (Table 5.3) was presumed for each field. Parcel A was not under BMP practices. Based on planted crop and nitrogen application rates of 2004 to

Table 5.4: Initial soil hydraulic parameters used. The top soil parameter values were taken as the Guelph Honeywood soil. (from Bekeris (2007).

Soil type	ρ_b(gr cm^{-3})	Sand (%)	Silt (%)	Clay (%)
Top-soil	1.10	20	55	25
Clay silt	1.98	35	45	20
Silt	1.72	5	85	10
Sandy silt	1.70	35	50	15
Silty sand	1.69	55	30	15
Fine sand	1.86	95	0	5
Sand/well-graded sand	1.74	90	0	10

2008, it was assumed that prior to 2003, Field A1 was under corn cultivation with nitrogen application of 90 and 60 kg ha^{-1} in May and June. Due to the indications of manure use, it was assumed that 4.75 ton ha^{-1} beef cattle manure with C:N ratio of 19 was being applied in April of each year to corn. This manure application is equivalent to 100 kg N ha^{-1} per year. Preliminary simulations showed that almost 30% of the manure is mineralized and becomes available to corn in the year of application. As a result, the total seasonal nitrogen application will become 180 kg ha^{-1} which is consistent with the recommended values (Table 5.3). It was assumed that the dominant cultivated crop on Fields B4 and B7 prior to 2003 was corn with seasonal nitrogen application of 90 and 60 kg ha^{-1} in May and June plus 100 kg N ha^{-1} of beef cattle manure. Also, it was assumed that occasional (once every 3 years) corn-soybean-winter wheat rotation was common during that time. Since winter wheat is planted after soybean, seasonal nitrogen application for winter wheat, presumed as 30 and 90 kg N ha^{-1} in October and April, was less than the minimum recommended value for hard red winter wheat (Table 5.3). Also, it was assumed that the recorded agricultural practices from 2003 to 2008 (Table 5.1) for these fields were continued until the end of the simulation period, 2012.

Since oat and grass parameters such as plant height, rooting depth and leaf area index are similar (Allen et al., 1998), grass was simulated as oat crop on Field

7B for 2005 to 2012. The detailed crop growth model, DSSAT was used for corn, soybean and Romano beans. DSSAT is parameterized for these crops. For other crops (Table 5.1) including winter wheat, red clover and oat, the Quickplant feature of the RZWQM was used.

For simulating soil nitrogen processes, soil organic matter background needs to be defined as an initial condition. Since no measurements of background soil organics, residues and inorganic nitrogen were available, these pools were equilibrated through a 15-year period simulation based on the historical agricultural practice prior to 2003 and soil condition at each station. For this simulation, the initial organic carbon of the upper most soil layer was adopted from Ecological Services for Planning (1996) for combined Honeywood and Guelph soil at the rate of 0.03 (gr OM gr^{-1}soil). The balanced pools determined at the end of this 15-year period simulation were used as the initial organic pools for each station.

5.2.3.3 Alternative BMP scenarios for Parcel A

Two plausible BMP scenarios were considered in accordance with the history of Field A1 and the common agricultural activities within the study site. In Scenario 1 corn is planted under reduced fertilizer application rate (30 and 80 kg N ha^{-1} in May and June). Scenario 2 included corn-soybean-winter wheat rotation with 30 and 80 kg N ha^{-1} application to corn in May and June, and 5 and 45 kg N ha^{-1} application to winter wheat in October and May. Manure rates in these scenarios were zero. The effect of these scenarios - if they had been applied in 1997- was simulated and compared to the current agricultural practice in Field A1 (Table 5.2).

5.2.3.4 Model Calibration and Validation

The purpose of model calibration was to adapt the RZWQM to the study field conditions, and then use the calibrated model to simulate the BMP effectiveness. Dynamically Dimensioned Search (DDS) optimization algorithm (Tolson and Shoemaker, 2007) was utilized. DDS is a stochastic single-solution based heuristic global

Table 5.5: Available field data for model calibration and validation (number of soil water content data points-number of soil nitrate concentration data points).

Stations	Soil core sampling dates					
	February 2005(1)	March 2005(1)	November 2005(1)	May 2006(1)	May 2007(2)	May 2008(2)
1(3)	-	-	Calib. (34-32)		Valid.(25-25)	
2	Calib. (62-66)			Valid.(52-52)		
6	Calib. (38-38)			Valid.(49-49)		
14	-	-	-	-	Calib. (45-45)	Valid. (40-40)
15	-	-	-	-	Calib. (30-30)	Valid. (25-25)

(1) from Bekeris (2007); (2) from Koch (2009); (3) 24 monthly water level data for Aquifer 2 from June 2005 to June 2008 are included

search algorithm. Three calibration trials each with different initial solution (generated randomly) and 250 model evaluations were performed. Selected soil hydraulic parameters (λ, ψ_b and K_{sat} of each soil layer), organic matter parameters (the fraction of organic matter that is transferred between fast residue to fast humus ($T_{f_r \to f_h}$), slow residue to intermediate humus ($T_{s_r \to i_h}$), fast humus to intermediate humus ($T_{f_h \to i_h}$) and intermediate humus to slow humus ($T_{i_h \to s_h}$) pools) and the seasonal nitrogen uptake by winter wheat (UPT_{ww}), red clover ($UPT_{redclov}$) and oat (UPT_{oat}) were calibrated for each station. For Station 1, the Aquifer 2 leakage rate was also calibrated.

Measured soil water content and nitrate concentration from several rounds of geologic cores were divided into two sections. The first split was used as the target of calibration and the second split was used to evaluate the performance of the calibrated model, so called model validation (Table 5.5). For Station 1, the Aquifer 2 water level recorded from June 2005 to June 2008 was also used as the calibration target. The root mean square error (RMSE) was used as the model calibration criteria to evaluate the simulation results, expressed as:

$$RMSE = W_{WT}\sqrt{\tfrac{1}{m}\sum_{i=1}^{m}\left(O_{WT,i}-S_{WT,i}\right)^2}+\sqrt{\tfrac{1}{n}\sum_{j=1}^{n}\left(O_{\theta,j}-S_{\theta,j}\right)^2}+\sqrt{\tfrac{1}{p}\sum_{k=1}^{p}\left(O_{NO_3,k}-S_{NO_3,k}\right)^2} \tag{5.1}$$

where WT is water table elevation (masl), θ is soil water content (%), NO_3 is soil nitrate concentration (mg $\mathrm{NO_3^-} - \mathrm{N}$ kg^{-1} soil), m is the number of water level observations, n is the number of θ observation, p is the number of soil nitrate measurements, O represents observed values, S represents simulated values, i is the i^{th} water level observation, j is the j^{th} θ observation and p is the p^{th} NO_3 observation. In this multi-criteria objective function, the magnitude of water level term was not comparable to the soil water and nitrate content terms over the range of parameter combinations and all observations. Therefore, a relative weight (W_{WT}) of 10 was assigned for water level elevation so that no criterion dominated the objective function.

In this study, the calibration range of the soil hydraulic parameters was determined from the RZWQM database (Rawls et al., 1998) in accordance to the soil class that was automatically assigned for each soil layer. The range of organic matter pool transformation rates were assigned to the maximum allowable limit (0-1). Typical nitrogen uptake for grain crops is 200 kg h^{-1}. The range of potential seasonal nitrogen uptake by winter wheat, red clover and oat was set to the typical value ± 50% (i.e., 100-300 kg ha^{-1}) (Table 5.6).

5.3 Results and Discussion

5.3.1 Parameter Calibration and Validation

For each recharge station, the parameter set associated with the calibration trial with the lowest RMSE was used. Most of the calibrated parameters were shared between different stations, and hence were calibrated in parallel (Table 5.6). For Stations 1 and 6, potential seasonal nitrogen uptake were calibrated as 247 and 223 kg ha^{-1} for winter wheat, 143 and 122 kg ha^{-1} for red clover and 178 and 154 kg ha^{-1} for oat. For Stations 1 and 6, the difference between calibrated potential nitrogen uptake by winter wheat and red clover (24 and 21 kg ha^{-1}, respectively)

Table 5.6: Calibrated parameters at Stations 1, 2, 6, 14 and 15.

Parameter		Unit	Calibration range	1	2	6	14	15
Top-soil (silty loam(1))	λ	-	0-0.492	0.15	0.44	0.17	0.28	0.18
	ψ_b	cm	0-168.0	48.31	42.09	33.52	37.2	28.67
	K_{sat}	cm hr^{-1}	0.32-1.43(2)	1.03	0.87	0.66	1.11	0.68
Clay silt (loam(1))	λ	-	0-0.584		0.37	0.32		
	ψ_b	cm	0-160.5		47.34	64.02		
	K_{sat}	cm hr^{-1}	0.39-3.40(2)		0.78	1.16		
Silt (loam(1))	λ	-	0-0.584				0.37	
	ψ_b	cm	0-160.5				38	
	K_{sat}	cm hr^{-1}	0.39-3.40(2)				1.38	
Sandy silt (loam(1))	λ	-	0-0.584					0.41
	ψ_b	cm	0-160.5					23.11
	K_{sat}	cm hr^{-1}	0.39-3.40(2)					1.41
Silty sand (sandy loam(1))	λ	-	0-0.854	0.36	0.36		0.32	
	ψ_b	cm	0-97.8	21.81	20.26		24.64	
	K_{sat}	cm hr^{-1}	1.30-5.58(2)	4.69	3.06		2.88	
Fine sand (sand(1))	λ	-	0-1.310			0.68		
	ψ_b	cm	0-47.4			12.4		
	K_{sat}	cm hr^{-1}	9.14-18.18(2)			18.16		
Sand/well graded sand (sand(1))	λ	-	0-1.310	0.73		0.59	0.59	0.81
	ψ_b	cm	0-47.4	11.15		7.04	18.12	20.19
	K_{sat}	cm hr^{-1}	9.14-18.18	14.51		18.16	15.51	18.16
$T_{f_r \to f_h}$		-	0-1	0.44	0.65	0.48	0.63	0.57
$T_{s_r \to i_h}$		-	0-1	0.71	0.85	0.63	0.83	0.76
$T_{f_h \to i_h}$		-	0-1	0.51	0.85	0.60	0.46	0.44
$T_{i_h \to s_h}$		-	0-1	0.77	0.23	0.70	0.68	0.56
UPT_{ww}		kg ha^{-1}	100-300	247	281	223		
$UPT_{redclov}$		kg ha^{-1}	100-300	143	186	122		
UPT_{oat}		kg ha^{-1}	100-300	178		154		
Aquifer 2 leakage rate		cm hr^{-1}	1E-010-1.0(3)	1E-003				

(1) soil class assigned by the RZWQM according to the specified soil particle sizes.; (2) Rawls et al. (1998); (3) based on minimum and maximum allowable limits.

was less than the difference for Stations 1 and 2 (34 and 43 kg ha^{-1}) and Stations 6 and 2 (58 and 64 kg ha^{-1}). These variations are a result of the differences between cropping rotation and nitrogen application of Field B4 and B7. Potential nitrogen uptake by winter wheat and red clover for Station 2 is considerably higher than Stations 1 and 6. This is likely due to the presence of higher nitrate content in the soil profile at Station 2 (241 kg ha^{-1} compared to 49 and 26 kg ha^{-1} at Stations 1 and 6 for 2003 to 2012) which is related to the finer soil material of the second soil layer at this station.

The calibrated parameters were employed for the RZWQM simulations. Resulting soil water content and nitrate concentration were compared for the validation dates (Table 5.5) in Figure 5.3 and Figure 5.4. Using calibrated RZWQM, soil water content was simulated with the RMSE of 6.7, 12.1, 7.0, 1.1 and 4.1% for all validation dates (listed in Table 5.5) for stations 1, 2, 6, 14 and 15, respectively. For these stations, soil nitrate concentration was simulated with the RMSE of 2.2, 3.9, 4.6, 9.0 and 2.3 mg $NO_3^- - N$ kg^{-1} soil, respectively. The simulated soil nitrate concentration within the top 20 cm of the soil profile was considerably underestimated for most validation dates (Figure 5.4); that is, 68% in May 2007 for Station 1; 98 and 68% in May 2006 and 2007 for Station 2; 73, 90 and 69% in May 2006, 2007 and 2008 for Station 6, and 36 and 50% in May 2008 for Stations 14 and 15, respectively. High nitrate concentration, measured in the top soil layer in spring (that is, May), can be an indication of either fresh nitrogen application or significant nitrate production as a result of soil organic matter decomposition. According to the available management information (Table 5.2), Field A1 received 112 kg N ha^{-1} in May; however, the exact date of application is not known. For modeling purposes, it was assumed that nitrogen application took place on May 01, 2008. Validation date in 2008 corresponds to the model simulation for May 10 which is 10 days after nitrogen application. However, in reality, it could have been possible that the sampling date for soil nitrate measurement was closer to the nitrogen application date (<10 days), and hence the measured nitrate in the upper soil layer was greater than the model estimates. However, this explanation is not valid for other stations because

Field B4 and B7 did not receive any fertilizer since April 2005 (Table 5.2). Also, it could have been possible that the initial soil organic matter at the beginning of the BMP simulation in January 2003 was underestimated. According to Seiter and Horwath (2004) the organic manure nitrogen not mineralized is integrated into the soil organic matter and becomes an important residual nutrient source in the later years. Finally, atmospheric deposition can be responsible for the high nitrogen content measured in the top 20 cm of the soil profile. According to Miller et al. (1990), nitrogen deposition is high in southern Ontario due to incoming pollutant from United States and high urbanization. Nitrogen deposition range is 16 to 25 kg ha^{-1} per year (Canadian Forest Service, 1999). The RMSE for the simulated soil nitrate content is 1.0, 1.9, 1.2, 9.0 and 0.6 mg $NO_3^- - N$ kg^{-1} soil for stations 1, 2, 6, 14 and 15, respectively, if the top 20 cm of the soil layer is ignored.

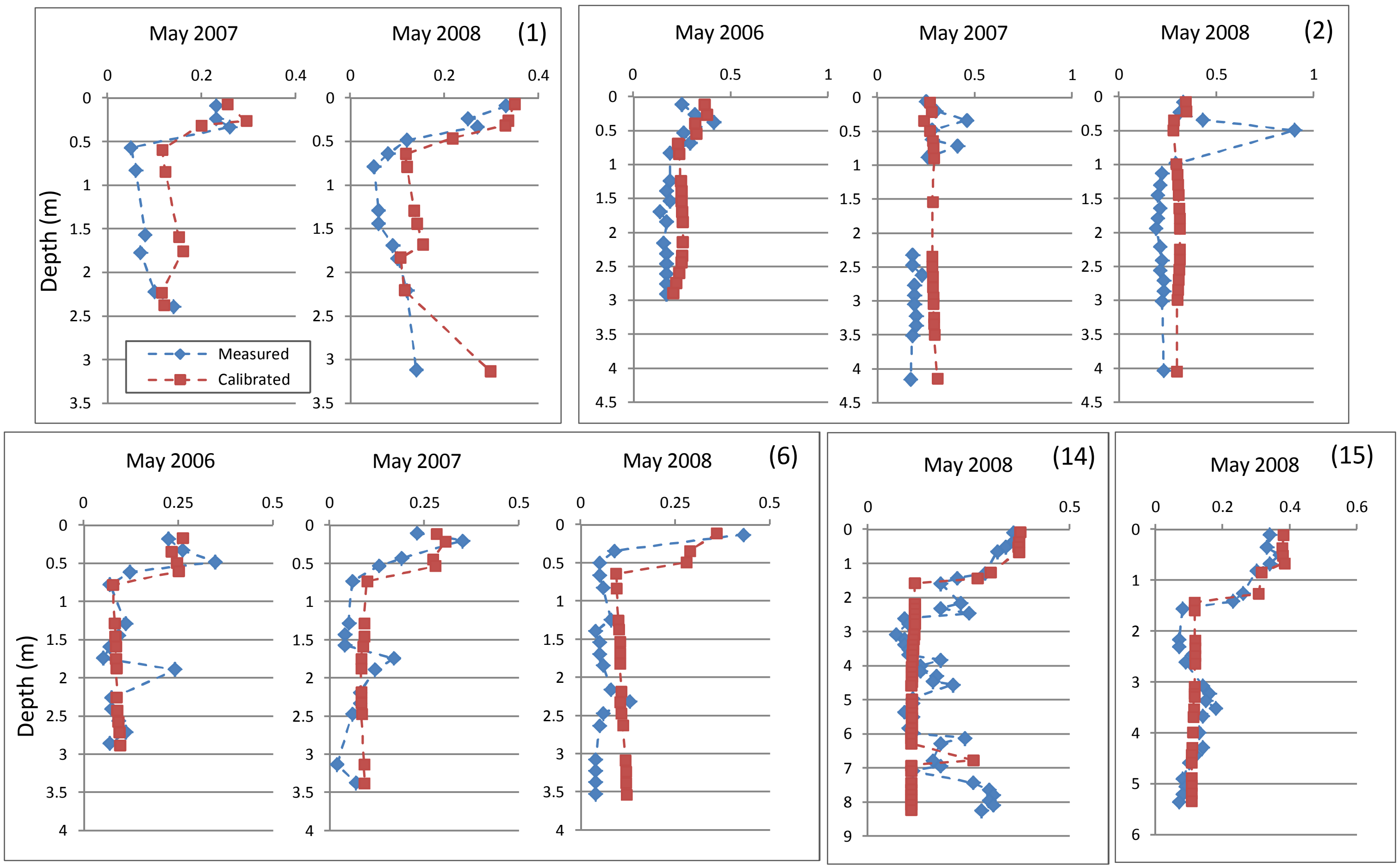

Figure 5.3: Measured and predicted volumetric soil water content (m^3m^{-3}) using the calibrated RZWQM at Stations 1, 2, 6, 14 and 15 for the validation dates.

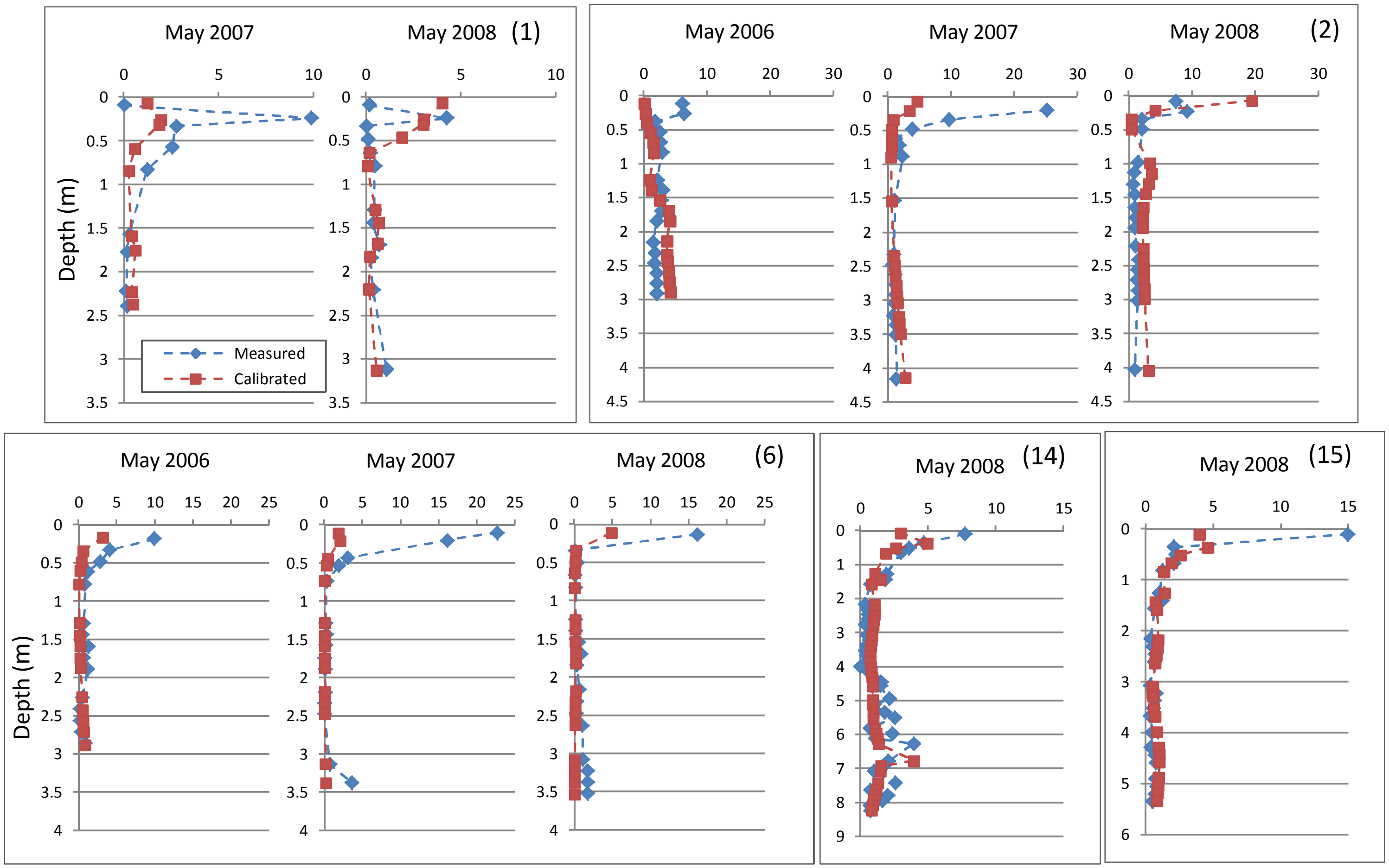

Figure 5.4: Measured and predicted soil nitrate concentration (mg $NO_3^- - N$ kg^{-1} soil) using calibrated RZWQM at Stations 1, 2, 6, 14 and 15 for the validation dates.

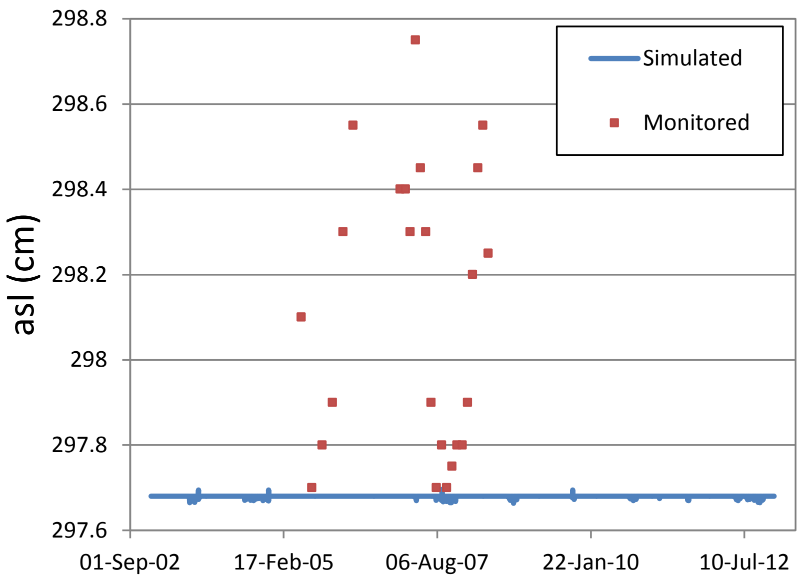

Figure 5.5: Simulated and measured Aquifer 2 water level at Station 1.

The lateral leakage rate of Aquifer 2 in Station 1 was calibrated to 1E-003 cm hr^{-1}. The calibrated RZWQM could not reproduce the observed fluctuations of the Aquifer 2 water level (Figure 5.5).

5.3.2 Groundwater Recharge and Nitrate Leaching Simulations

Nitrate mass flux, simulated by the calibrated RZWQM, was underestimated by 23 and 38% for Stations 1 and 6 during May 2005 to May 2006, and 63, 85, 70 and 31% for Stations 1, 6, 14 and 15 during May 2007 to May 2008. But, nitrate mass flux during these time periods was overestimated by 222 and 30% for Station 2 (Figure 5.6). Groundwater recharge was estimated at 51, 37 and 46 cm for Stations 1, 2 and 6 during May 2005 to May 2006, and 18, 24, 20, 37 and 31 cm for Stations 1, 2, 6, 14 and 15 during May 2007 to May 2008. That is equivalent to 19, 77 and 6% overestimation for Stations 1, 2 and 6 during May 2005 to May 2006, and 64, 43, 62, 45 and 36% underestimation for Stations 1, 2, 6, 14 and 15 during May 2007

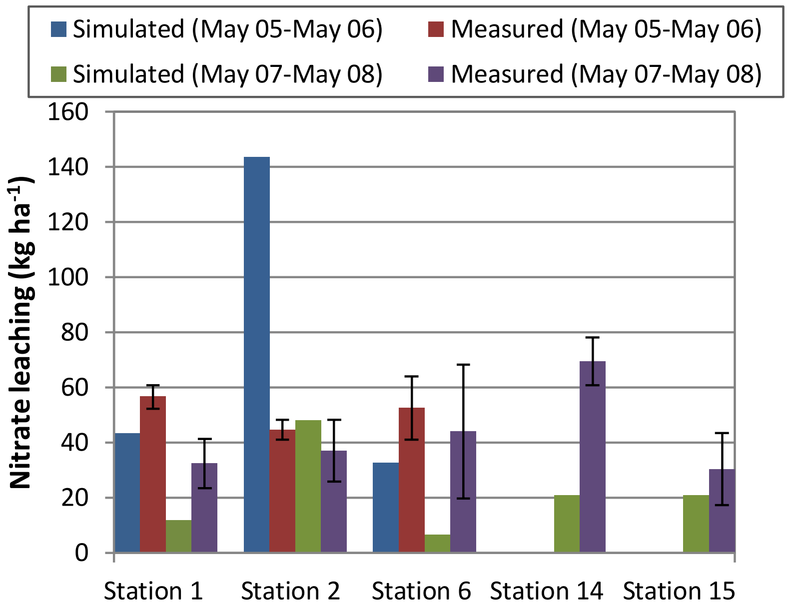

Figure 5.6: Comparison of simulated and field-estimated (with upper and lower estimation bound) nitrate mass load using calibrated RZWQM for Stations 1, 2, 6, 14 and 15.

to May 2008 (Figure 5.7).

The upper and lower bounds of field recharge estimates were determined from the standard deviation of the soil water content measurements within the spatial and temporal intervals of tracer migration below 0.3 m (Bekeris, 2007) (Figure 5.7); that is May 2006 cores for May 2005-May 2006 and May 2008 cores for May 2007-May 2008 periods. For nitrate mass flux, the upper and lower bounds of the field estimates were calculated from the standard deviation of both groundwater recharge and soil nitrate concentration (Figure 5.6). Groundwater recharge and nitrate mass flux simulated by the RZWQM for the periods of May 2005-May 2006 and May 2007-May 2008 were mostly out of field-estimated bounds, suggesting that the simulations were associated with error. However, several sources of potential uncertainties related to the soil coring technique could result in significant spatial and temporal variations in recharge estimates (Koch, 2009). One significant drawback of the field estimated recharge, calculated by Bekeris (2007) and

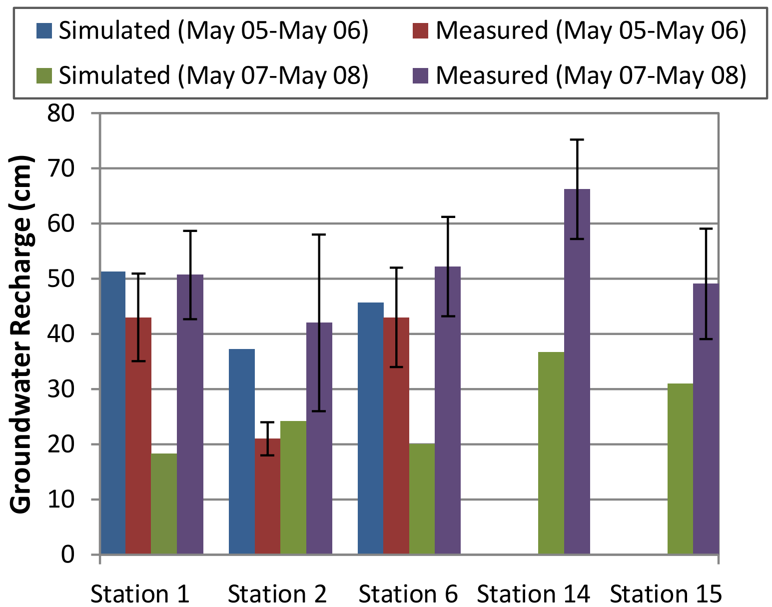

Figure 5.7: Comparison of simulated and field-estimated (with upper and lower estimation bound) groundwater recharge using calibrated RZWQM for Stations 1, 2, 6, 14 and 15.

Koch (2009), was the assumption they made to scale a yearly rate of recharge from the limited observed tracer migration data. That is, the average monthly recharge rate estimated from the observed tracer migration, which was 9.5 months for May 2005-May 2006 (Bekeris, 2007) and 4 months for May 2007-May 2008 (Koch, 2009) was adopted as the average monthly rate for missing months, and therefore the tracer migration over observed months were scaled proportionally to one year. The yearly recharge rate extrapolated with this assumption might be defective; particularly for the period from May 2007 to May 2008 for which observed tracer migration months were limited to the wet and cold months of the year (i.e., January to April). As a result yearly recharge rate could have been overestimated. This can explain the significant underestimation of recharge, simulated by the RZWQM during May 2007-May 2008 (Figure 5.7). Since recharge is one of the two factors in nitrate mass load calculation, overestimating recharge would have affected field estimated nitrate leaching.

On average, 17% of water flux at Station 1 during 2003 to 2012 is upward flow with a maximum value of 8 cm during 2012. As the result of this upward flow, on average, 1.9 kg ha^{-1} nitrate moved upward into the soil profile. The maximum rate of upward nitrogen flow occurred at the rate of 6.5 kg ha^{-1} during 2007. The upward water flux and nitrogen flux in 2005 and 2006 was zero. According to the RZWQM simulation results, a total of 10.0 kg ha^{-1} nitrate was lost to lateral flow of Aquifer 2 at Station 1 during 2003 to 2012.

5.3.3 BMP Effectiveness for Parcel B

Annual nitrate leaching from Fields B7 and B4 are presented in Figure 5.8 for 2003 to 2012. Nitrate leaching varied significantly for different years ranging from 3.4 to 93.5 kg ha^{-1} for Station 1, 2.1 to 55.1 kg ha^{-1} for Station 6, and 28.3 to 222.2 kg ha^{-1} for Station 2. This is a result of variation in weather, soil organic matter residue, and cropping and nitrogen application rate.

Nitrate leaching decreased immediately after BMP implementation; i.e., from 43.0, 42.3 and 190.8 kg ha^{-1} for Stations 1, 6 and 2, averaged for 2000 to 2002 (three years prior to BMP activation) to 22.4, 23.4 and 148.2 kg ha^{-1} averaged for 2003 to 2005 (three years after BMP activation). This is equivalent to 48, 45 and 22% reduction in nitrate leaching for Stations 1, 6, and 2, respectively.

To demonstrate the benefit of BMP implementation, nitrate mass flux was simulated for 2003 to 2012 as if historical management practice would have been continued (no BMP), and results were compared. Averaged annual nitrate mass load under BMP was 24.1, 16.4 and 101.0 kg ha^{-1} for Stations 1, 6 and 2 from 2003 to 2012. If BMP management had not been implemented, this would have been 28.8, 35.3 and 91.5 kg ha^{-1} for the same period of time. This means nitrate mass loading, on average, was reduced by 16 and 54% over a 10-year period after BMP adoption for Stations 1 and 6, whereas it increased by 9% for Station 2. This suggests that BMP was more effective on reducing nitrate load at Stations 1 and 6 than Station 2.

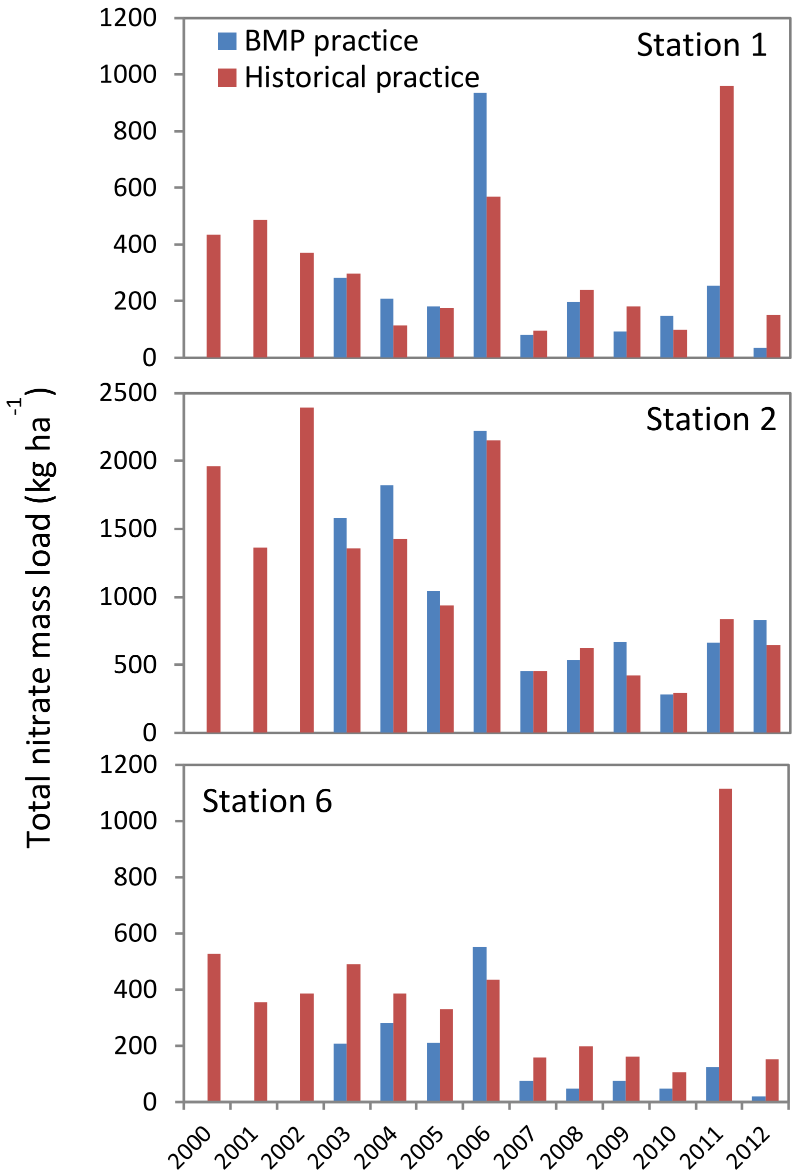

Figure 5.8: Simulated nitrate mass load using calibrated RZWQM under BMP and historical agricultural practices for Stations 1, 2 and 6.

Figure 5.8 clearly shows that the simulated annual post BMP nitrate mass loading is not necessarily less than the simulated nitrate mass loading before BMP activation. For instance, nitrate mass loading for 2006 under BMP conditions was predicted to be 54 and 23% more than average nitrate loading for 2000 to 2002 (three years prior to BMP adoption) for Stations 1 and 6, respectively. This simulation result conforms to the unexpected increase in post BMP mass load during 2005 and 2006 reported by Bekeris (2007), and suggests that BMP effectiveness needs to be investigated over a long period of time and single field measurements cannot address the impact of BMP on nitrate leaching.

In Figure 5.9, the annual nitrate mass load, and average daily soil nitrate content are shown for 2003 to 2012. The Spearman Rank-Order Correlation Coefficient was calculated to assess the relationship between these two variables at Station 1, 6 and 2. The coefficient was calculated as 0.48 0.71 and 0.52 (for df = 8, a correlation coefficient of 0.74 is required for statistical significance at 0.05 level). Hence, although there is a positive agreement between nitrate load and soil nitrate content; there is no significant relationship between these two variables. And hence, the reduction of soil nitrate content compared to its previous year does not necessarily imply that nitrate leaching has been reduced.

5.3.4 Anticipated BMP Impact for Parcel A

The annual nitrate mass loading simulated under current agricultural practices (Table 5.2) for the period of 1997 to 2012 ranges from 1.4 to 96.4 kg ha^{-1} for Station 14, and 1.7 to 117.4 kg ha^{-1} for Station 15 with an average of 40.9 and 40.8 kg ha^{-1} for these two stations. Average nitrate mass loading simulated under BMP Scenario 1 (i.e., only corn) and Scenario 2 (i.e., corn-soybean-winter wheat rotation) was reduced to 26.1 and 31.6 kg ha^{-1} for Station 14 and 23.6 and 29.5 kg ha^{-1} for Station 15. This suggests that BMP Scenario 1, on average, can reduce the nitrate load (36 and 42% for Stations 14 and 15) more than BMP Scenario 2 (23 and 28% for Stations 14 and 15) during 16-year period (Figure 5.10).

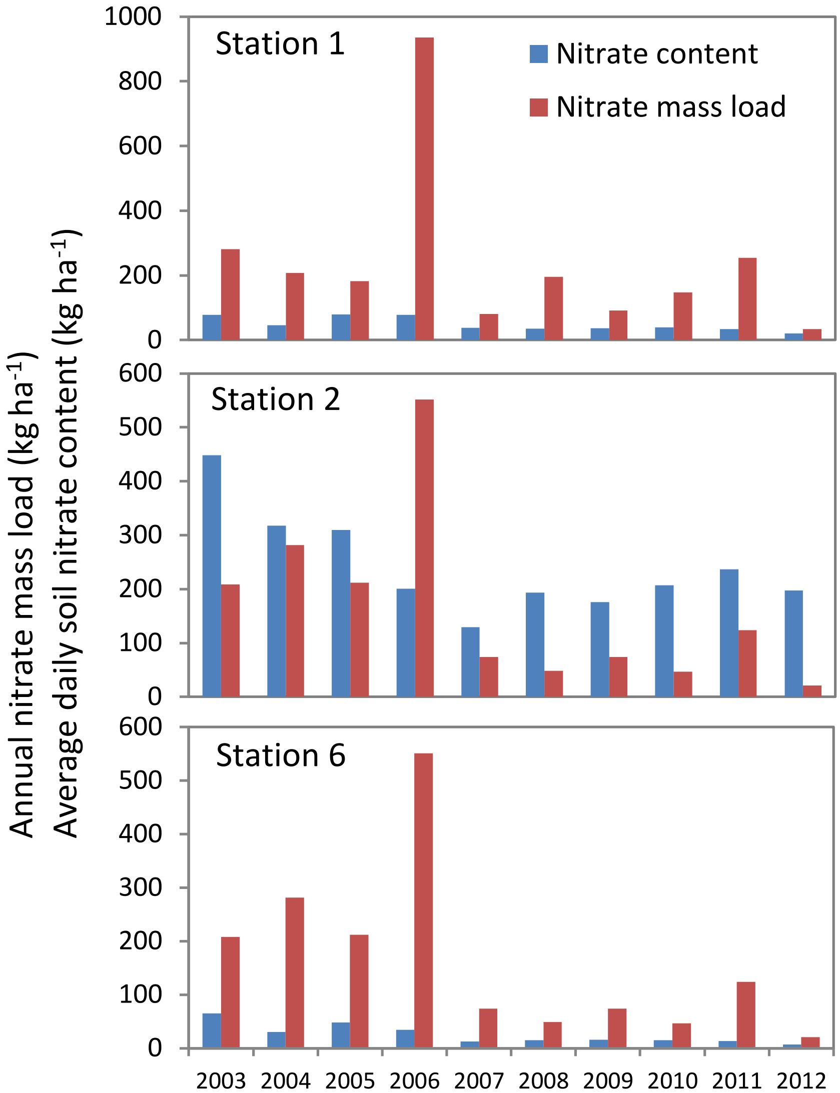

Figure 5.9: Simulated annual nitrate mass load and average daily soil nitrate content using the calibrated RZWQM under BMP and historical practices for Stations 1, 2 and 6.

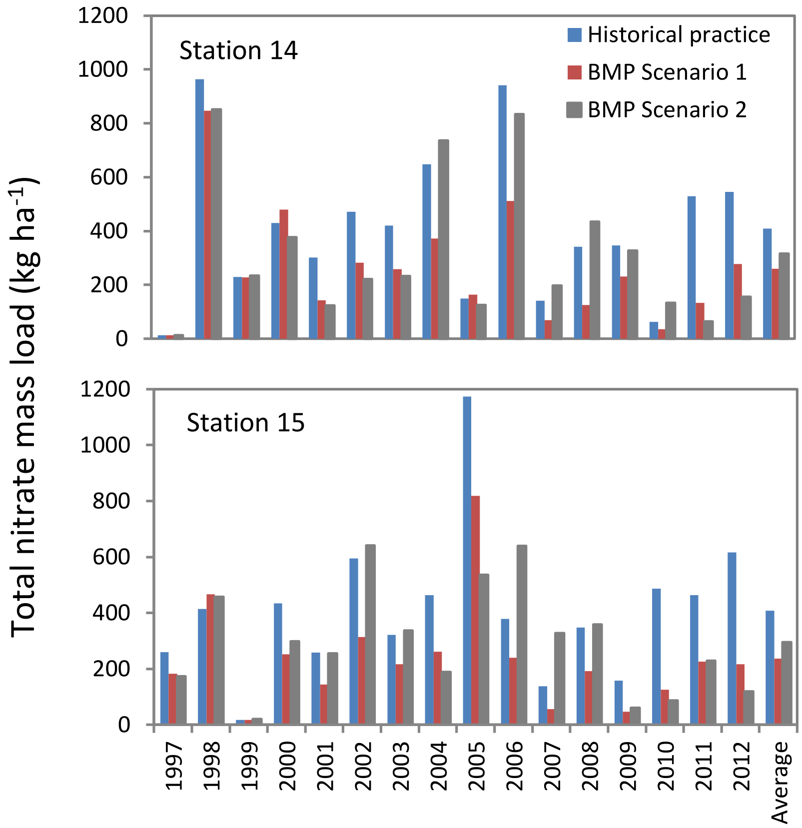

Figure 5.10: Simulated nitrate mass load using the calibrated RZWQM under historical and BMP Scenarios 1 (corn) and 2 (corn-soybean-winter wheat) practices for Stations 14 and 15.

The initial soil nitrate concentration on January 01, 1997 was simulated as 218 and 120 kg ha^{-1} for Stations 14 and 15. The final soil nitrate content on December 30, 2012 was 71 and 97 kg ha^{-1} for BMP Scenarios 1 and 2 for Station 14, and 44 and 75 kg ha^{-1} for Station 15. Linearly, simulated soil nitrate content at Station 14 was reduced at the rate of 7.7 kg ha^{-1} per day for both Scenarios 1 and 2, whereas for Station 15 the reduction rate was 4.9 and 3.2 kg ha^{-1} per day for Scenarios 1 and 2, respectively (Figure 5.11). Even though the nitrogen application for the BMP management was less, simulated soil nitrate content under these BMP scenarios exceeded the current agricultural practices' soil nitrate content (Figure 5.11). This occurrence during the first years after BMP implementation was predicted to be more frequently and significantly. This supports the view that BMP effectiveness cannot be evaluated from single measurements of soil nitrate content, particularly when evaluation is immediate after BMP adoption, and long-term assessment is required.

Simulated seasonal nitrogen uptake by corn, which is the common crop for the current practice and BMP Scenarios 1 and 2, was compared for the three conditions. In the early years after BMP implementation, simulated nitrogen uptake by corn under the current practice was slightly greater than uptake under the two BMP Scenarios (e.g. 2%, on average, for 1997 in Station 15) but in the last year of simulation, N-uptake in Scenario 2 becomes the greatest (e.g., 7 and 19% more than the current practice and Scenario 1 for 2012 in Station 15) (Figure 5.12). This increase can be a side benefit of the significant contribution of soybean to soil nitrogen supply through nitrogen fixation (i.e., 967 and 970 kg ha^{-1} during 16-year simulation period for Station 14 and 15, respectively, for five soybean rotations) (Figure 5.13). Overall, N-uptake by corn was not reduced under BMP conditions and is comparable with the current practice.

For the current practice, losses from denitrification (1021 and 1062 kg ha^{-1} for Stations 14 and 15) and volatilization (644 and 642 kg ha^{-1} for Stations 14 and 15) were simulated to be significantly more than Scenario 1 and 2. For the current agricultural management practice, soil nitrogen storage was increased at the rate of 759 and 800 kg ha^{-1} during the simulation period likely due to the manure application. Under BMP practices soil nitrogen storage was significantly less, even being negative (-52 kg ha^{-1}) at Station 14 for BMP Scenario 1 (Figure 5.13). Even though nitrate leaching in Scenario 1 was less than Scenario 2, the total nitrogen loss (i.e., denitrification + volatilization + leaching) for Scenario 2 was 17% less than Scenario 1 for both stations, suggesting that the overall nitrogen management in Scenario 2 was better than Scenario 1 (Figure 5.13).

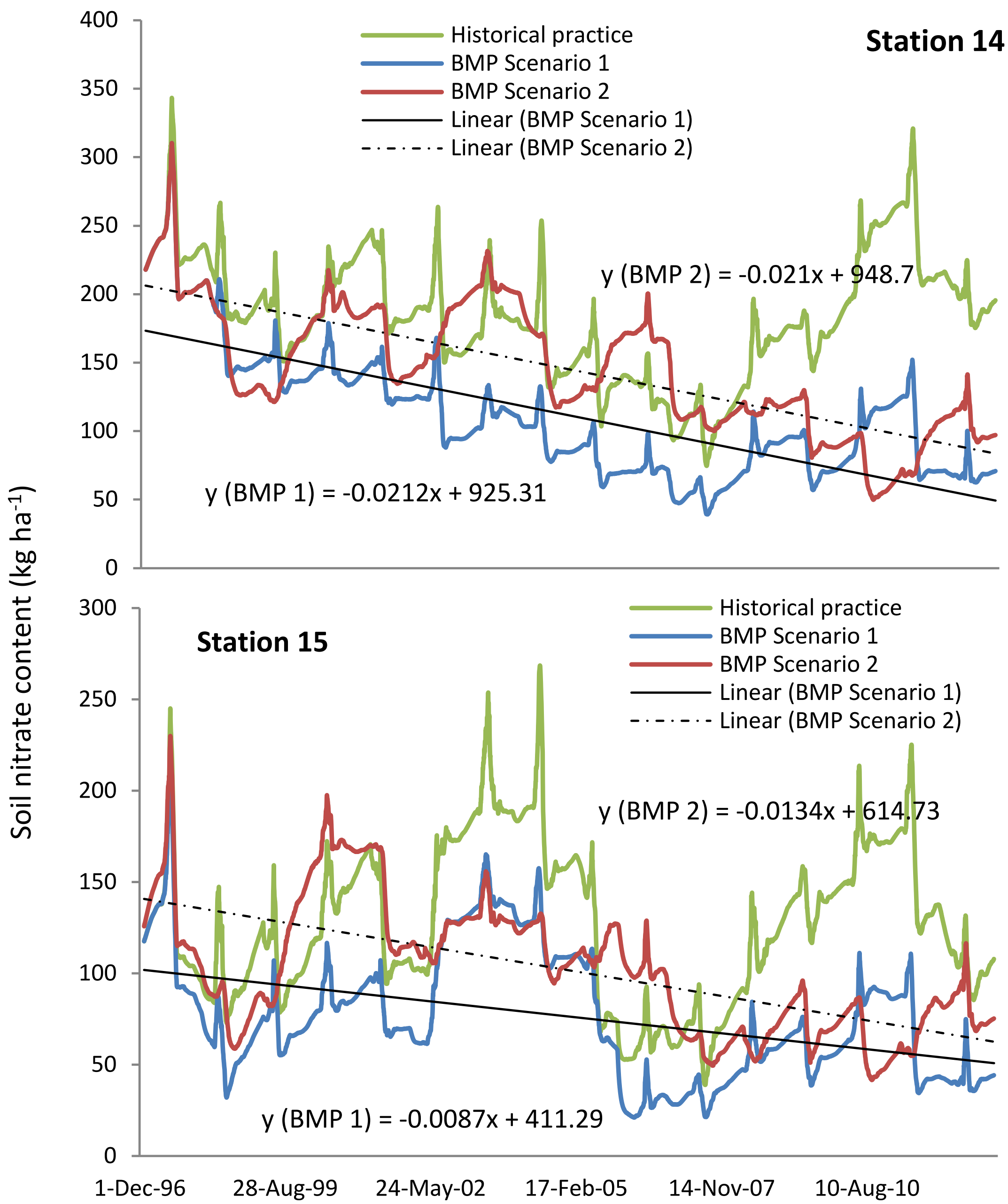

Figure 5.11: Simulated soil nitrate content using the calibrated RZWQM under historical and BMP Scenarios 1 (corn) and 2 (corn-soybean-winter wheat) practices for Stations 14 and 15.

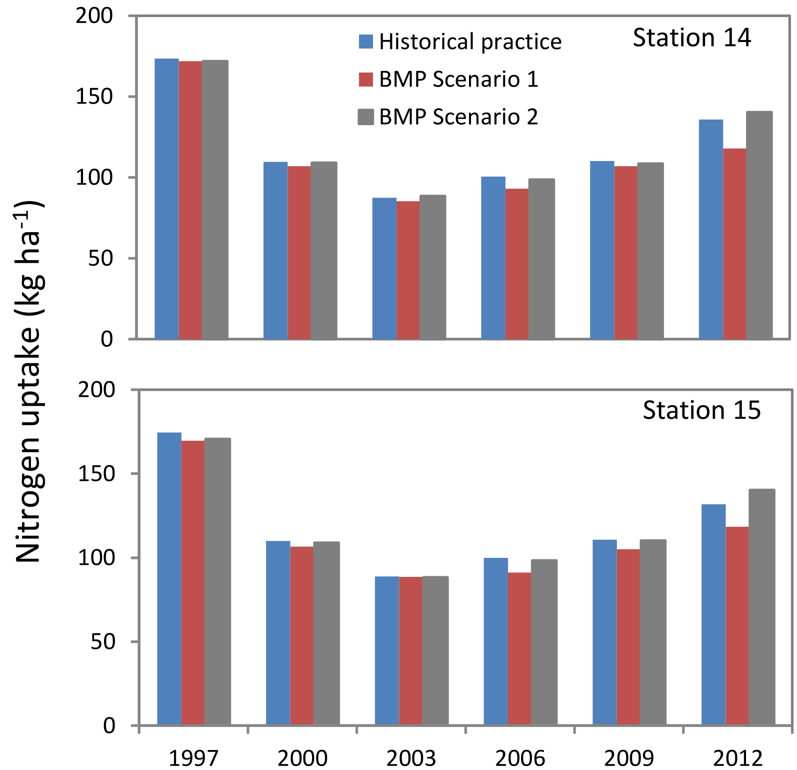

Figure 5.12: Simulated nitrogen uptake by corn using the calibrated RZWQM under historical and BMP Scenarios 1 (corn) and 2 (corn-soybean-winter wheat) practices for Stations 14 and 15.

5.4 Conclusion

In this study the RZWQM was calibrated to the soil water content and nitrate concentration data obtained from five different locations including Stations 1, 2, 6, 14 and 15 across the Woodstock Well Field. The calibrated model was able to represent these observations within the soil profile at different stations for the validation dates. That is, volumetric soil water content was estimated with RMSE ranging from 1.1 to 12.1% for Stations 14 and 2, respectively. The range of RMSE for soil nitrate concentration was 2.2 to 9.0 (mg $NO_3^- - N$ kg^{-1}soil) for Stations 1 and 14. Soil nitrate concentration within the top 20 cm of the soil profile was considerably underestimated for most validation dates. High nitrogen concentration, measured

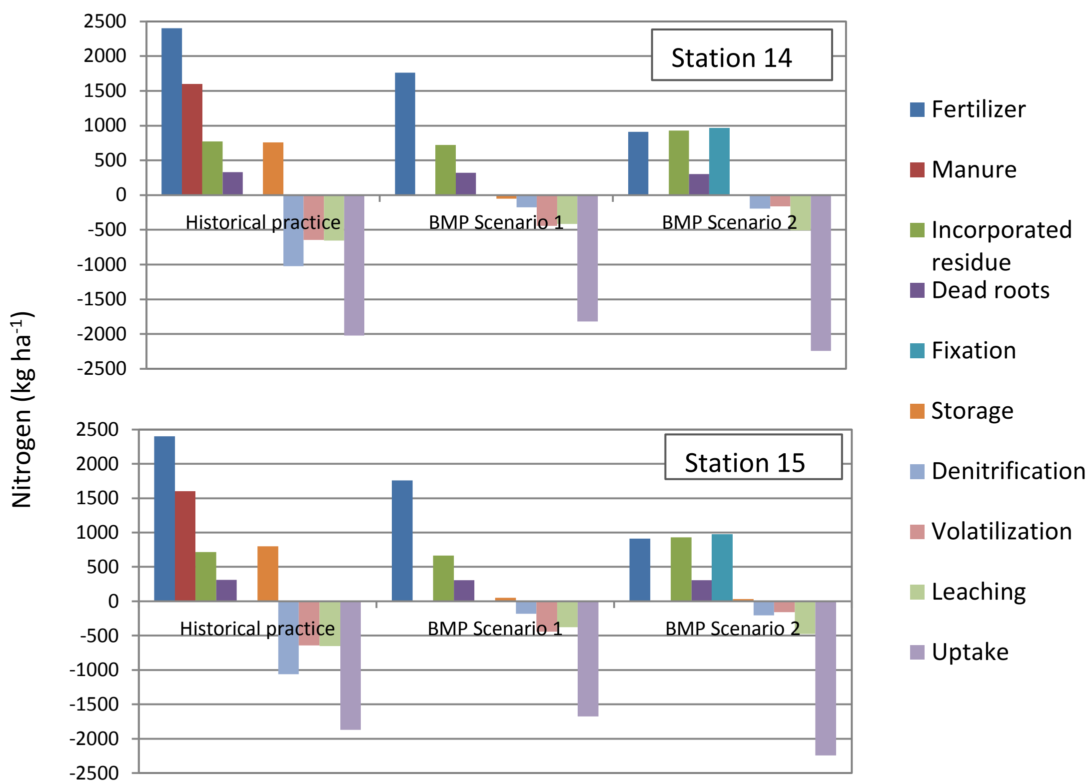

Figure 5.13: Nitrogen addition and losses predicted by the calibrated RZWQM under historical and BMP Scenarios 1 (corn) and 2 (corn-soybean-winter wheat) practices for Stations 14 and 15.

in the top soil layer was likely related to recent nitrogen application in May (only for Stations 14 and 15) or significant atmospheric nitrogen deposition which was not accounted by the model. Also, it could have been possible that the soil organic matter content initiated at the start of the simulation was underestimated.

Using calibrated RZWQM, simulated groundwater recharge and nitrate leaching for the periods of May 2005-May 2006 and May 2007-May 2008 were mostly out of field-estimated bounds, suggesting that groundwater recharge and nitrate leaching were simulated with error. However, the performance of the model could not be evaluated due to the uncertainties associated with the measurement techniques and calculation assumptions.

According to the modelling results, the BMP effect on nitrate leaching was immediate. That is, average nitrate leaching over three years after BMP implementation compared to three years before BMP activation was reduced by 48, 45 and 22%, respectively, for Stations 1, 6, and 2.

Post BMP nitrate load was simulated as not necessarily being less than before BMP activation nitrate leaching. This simulation result can explain the increase in the Woodstock supply wells' nitrate concentration, observed since 2003. As suggested by Inamdar et al. (2001), increasing nitrate load after BMP application was likely due to the ammonification, nitrification, and subsequent leaching of the conserved organic nitrogen in the soil profile. The fluctuation of nitrate load can also be the result of variation of other factors, such as precipitation and temperature that controls nitrate transformation and transport. It is suggested that BMP effectiveness needs to be investigated over a long period of time and single field measurements cannot address the BMP impact on nitrate mass load.

The Spearman Rank-Order Coefficient was used to interpret the correlation between annual nitrate load and soil nitrate content for Parcel B for after BMP implementation. It was concluded that there was a positive agreement between nitrate load and soil nitrate content; however, no significant relationship was found between these two variables. And hence, the reduction of soil nitrate content compared to its previous year does not necessarily imply that nitrate load has been reduced.

Overall, the findings of this study indicate that the BMPs were effective in reducing nitrate load from Parcel B farmlands into the groundwater; however, more time is needed to observe significant response to the BMPs in Field B4.

The effects of two alternative BMP scenarios on Parcel A were modeled. In Scenario 1, only corn is planted under reduced fertilizer application rate, whereas Scenario 2 included corn-soybean-winter wheat rotation. Both Scenarios were under reduced fertilizer and zero manure application. Implementation of Scenario 1, on average, was predicted to reduce nitrate load (36 and 42% for Stations 14 and 15) more than BMP Scenario 2 (23 and 28% for Stations 14 and 15) during a 16-year period. Even though nitrate mass load in Scenario 1 would be less than Scenario 2, the total loss of nitrogen (denitrification + volatilization + leaching) for Scenario 2 was 17% less than Scenario 1 for both stations, suggesting that the overall nitrogen management in Scenario 2 was better than Scenario 1. According to the model simulations, nitrogen uptake by corn planted in Parcel A is not reduced under BMP practices and is comparable with the current agricultural practice.

Chapter 6

Closure

6.1 Conclusions and Contributions

The main objective of this study was to evaluate the performance of two research-level agricultural nitrogen models; RZWQM and CoupModel to simulate nitrate leaching below the root zone. Prior to this evaluation, the influential parameters of each model were calibrated and validated using a set of field data to yield each models' maximum prediction capacity. A global sensitivity analysis was performed to identify the influential parameters of the RZWQM, whereas the calibrating parameters of the CoupModel were selected based on available literature values. The focus of this study was on both water flux, which directly governs solute transport in the soil profile, and overall nitrate leaching. Accordingly, model calibration and validation were handled in a step-wise fashion on these model components. The successful model/sub-model was determined. In this study also, the transportability of a successfully calibrated and validated model to simulate water flow and nitrate leaching in a location other than the calibrating site with similar agricultural and environmental conditions was tested. Finally, the effectiveness of a long-term-implemented BMP to reduce nitrate leaching was investigated using an agricultural nitrogen model tool.

The major conclusions emerging from this research and significant contributions to the field of nitrate leaching modeling are listed below.

- The sensitivity analysis was performed for the RZWQM with the data from an experimental raspberry farm in Abbotsford, BC. The influence of 70 parameters including 35 hydrological parameters and 35 nitrogen cycle parameters were tested over various vertical-spatial and temporal domains. In this study, not only the parameters' importance was ranked, but also the contribution of individual input parameters to the output uncertainties was apportioned. The investigated soil profile consisted of three soil layers which the third one was recognized as the top of the aquifer. Briefly, bulk density for soil Layer 1, field capacity for soil Layers 1 and 3 and albedo of the crop were the key parameters affecting water flux and ET. The parameters that had the most influence on the following nitrogen-related outputs: total $NO_3^- - N$ in the soil profile, mineralization, denitrification loss, nitrate leaching and plant N-uptake were the transient coefficient of fast to intermediate humus pool; C:N ratio of the fast humus pool; organic matter decay rate of fast humus pool; and field capacity for Layer 3.

- None of the investigated RZWQM outputs were found to be sensitive to the macroporosity parameters (17 parameters) for which the maximum allowable range by the model was tested. This finding was related to the inability of the RZWQM macroporosity model (i.e., gravity preferential model) to account for the preferential flow in a sandy soil profile.

- The correlated contribution of studied parameters to the model outputs uncertainties was $< 10\%$. If these small correlations are neglected, the investigated RZWQM parameters can be considered as independent, and hence their contributions to the uncertainty in the model outputs can be studied independently; that is, local sensitivity analysis techniques are applicable.

- It was found that calibrating an excessive number of RZWQM hydrological parameters (35 parameters) increased the risk of over-parameterization and deteriorated model predictions. Using sensitivity analysis results, the number of parameters that required calibration was minimized from 35 parameters to as few as four parameters, for which even manual calibration is applicable. This finding reduces the burden of applying sophisticated automatic calibration methods.

- The field observations that have the most shared sensitive parameters with the model output of interest are most effective to use as RZWQM calibration targets. Quantitative sensitivity analysis results can be used to investigate not only the most sensitive parameters that effect the output of interest but also the location and time of the field observations that share those sensitive parameters with the output of interest, and hence to design experimental studies to yield the investigated observations. Under the current study conditions, average soil moisture content over the upper 30 cm of the soil profile was the most effective moisture observation (compared to the moisture data at other depths) to use as the calibration target when the goal of calibration is to improve water flux prediction from March to October.

- For the calibration, validation and comparison of the RZWQM and CoupModel, a step-wise approach was developed in Chapter 3, based on parameter requirements of each model and available field data on raspberry rows and inter-rows from the experimental raspberry farm in Abbotsford, BC. That is, first, selected soil hydraulic parameters were calibrated. Then, data from the raspberry inter-rows which were free of vegetation and nitrogen application were used for the modification of the seasonal nitrogen mineralization and soil organic matter parameters. Finally, selected growth parameters of the raspberry crop were calibrated. Through these processes, two important nitrogen sink and source terms (i.e., mineralization and N-uptake) were identified.

- Calibration of the RZWQM hydraulic parameters via DDS optimization algorithm improved water flux estimation by 37% when compared to the estimations obtained from model default hydraulic parameter which were recommended based on soil texture, whereas for the CoupModel, water flux estimations obtained from the calibrated hydraulic parameters, using the GLUE optimization algorithm, did not improve compared to the results from model's recommended values which were determined from a pedo-transfer function. This suggested that under current study conditions calibration of RZWQM hydraulic parameters in order to improve water flux estimation is worth the time and effort, but not for the CoupModel.

- Water flux time plots simulated by both calibrated RZWQM and CoupModel were in reasonable agreement with field observations; however, calibrated RZWQM rather outperformed the CoupModel by 22%. The superior performance of the RZWQM was found to be related to both using a more efficient calibration algorithm (i.e., DDS) and application of a better ET model.

- In contrast to water flux estimations, the CoupModel simulated nitrate leaching time series better than RZWQM. This finding was related to the application of more inclusive growth models in CoupModel (i.e., the logistic and the water use efficiency approaches) in comparison to the RZWQM which only mimics growth when woody species such as raspberries are modeled.

- Simulated nitrate leaching time series was strongly correlated with water flux estimations due to the high permeability of the soil profile in Abbotsford BC, suggesting that the error associated with water flux simulation can readily be transferred to the nitrate loading simulations. This, however, was not consistent with the overall findings of Chapter 3 that the CoupModel simulated water flux less well compared to the RZWQM, while it outperformed RZWQM for simulating nitrate leaching. This occurrence was related to the flexibility of the CoupModel which allowed for changes in soil organic matter and growth parameters, as the result of calibration, to compensate for error associated with water flux and solute transport simulation. This effect, known as "parameter lumping" (Dubus et al., 2002), may thus result in an increase in the soil organic matter and growth parameters' uncertainties, although may not be perceptible by the model user.

- The logistic growth approach of the CoupModel and the Qcktree module of RZWQM both use potential N-uptake parameter. According to the findings of this study, this parameter which has a great influence on overall soil nitrogen balance is highly sensitive to the variation of irrigation and nitrogen applications. Hence, one single value does not address all agricultural practices, and calibration of this parameter is critical when RZWQM or CoupModel with the logistic growth approach is used. Potential N-uptake parameter, however, is not required when the water use efficiency approach of the CoupModel is used. This approach only requires the identification of the water use efficiency parameter which is constant for a specific plant and climate condition. Hence, this growth approach was found to be more robust for the simulation of plant growth when the CoupModel is used. Under the current study conditions, an average value of 5.13 (μ mol CO_2 mmol^{-1} H_2O^{-1}) was obtained for water use efficiency parameter for raspberry crop.

- Overall, information about soil organic matter and growth parameters are vital for reliable application of both models. With such information, the CoupModel and the RZWQM (to less extent) were found to be reliable tools to simulate nitrate loading into the groundwater.

- The capability of the calibrated and validated CoupModel with water use efficiency approach used as the growth model was tested for simulating water and nitrate fluxes below the raspberry root zone in a commercial raspberry farm located within the Abbotsford region. The results of this investigation which were presented in Chapter 4 indicated that the transported model simulated seasonal water flux with 24% error; however, applications of the locally measured hydraulic parameters did not reduce this simulation error. Also, The transported CoupModel, simulated nitrate flux with an error of 104%; however, application of locally-measured hydraulic parameters reduced this error only by 17%. The discrepancies between simulated and field-measured water and nitrate fluxes were related to the inaccuracy of the management data of the commercial farm used as the model input data and/or the lack of CoupModel ability to account for the influence of the management of the raspberry inter-rows on nitrate and water flux on the raspberry row cropping system.

- The variability of the soil hydraulic parameters across the 15-ha commercial raspberry farm had minor influence on water flux estimation, and thus the transported hydraulic parameters can be used as a substitute for local values if not available to simulate seasonal water flux across this landscape. The variability of soil hydraulic parameters influence nitrate flux by up to 28% for the year in which manure is applied to the farm, suggesting that the mineralization of organic manure is sensitive to the variability of soil hydraulic parameters. Therefore, transported hydraulic parameters cannot be used as a substitute for the local values for the condition when organic matter applied to the soil is fresh and labile.

- The transported model can be considered as a useful tool for preliminary analysis of water and nitrate fluxes from the raspberry root zone for regional scale; but for further local analysis across the Abbotsford landscape, model parameters must be redefined from a sound scientific footing. The general concept of model transportability and the approach used to investigate it, in this study, is applicable for other physiographical regions in which some levels of similarity exist between different parcels within the region. A transported model is useful to investigate overall impact of nitrogen management on groundwater, and to support regional farming practices and policy options.

- Selected soil hydraulic, organic matter and growth parameters of the RZWQM were calibrated to a set of field data obtained from different locations at the Woodstock well Field and used to simulate groundwater recharge and nitrate leaching. Simulated ground water recharge and nitrate leaching by the calibrated RZWQM were mostly associated with error compared to the field-estimated bounds; however, the performance of the model could not be evaluated due to the significant uncertainties associated with the measurement techniques and calculation assumptions.

- According to the simulation results, implementing BMPs reduced nitrate leaching from Parcel B farmlands into the groundwater for up to 54% over a ten-year period after its adoption as the farming practice; however, this reduction was considerably variant at different station-locations.

- It was found that post BMP nitrate load is not necessarily less than before BMP activation nitrate leaching due to the complexity of nitrogen transformation and resultant nitrate leaching. Therefore, BMP effectiveness needs to be investigated over a long period of time and single field measurements cannot address the BMP impact on nitrate mass loading.

- The reduction of soil nitrate content compared to its previous year does not necessarily imply that nitrate load has been reduced; therefore, trends in soil nitrate concentration cannot be used as an index for BMP effectiveness, particularly for short period evaluations.

- Findings of this study provide an overall systematic approach for nitrogen modeling with the goal of nitrate leaching assessment when starting with a fresh site. The first step for such investigation would be selecting an appropriate simulation model based on required process details. It is suggested to perform sensitivity analysis in the second step in order to design appropriate experiments for collecting data and to define influential parameters. Next is model calibration and validation which warrant proper simulation results for local conditions. Such model can then be applied for transportability analysis and BMP assessment.

6.2 Recommendations for Future Works

- More effective calibration of soil hydraulic parameters and further characterization of plant development and carbon allocation parameters are recommended when using CoupModel as these practices are expected to improve simulation of nitrate leaching more. For the RZWQM, an inclusive growth model needs to become available for the simulation of woody species such as raspberry to obtain better nitrate leaching estimations.

- CoupModel is a one-dimensional model and simulates processes for a unit of area with single crop pattern. Therefore, combined simulation of the raspberry crop on rows and cover crop on inter-rows is not feasible. Development of modeling tools that can account for the interaction of these two cropping systems on overall nitrate leaching from the raspberry field is recommended.

- Overall, transported model was found as applicable to the conventional farm for simulating seasonal water flow and nitrate flux (except for the year in which manure was applied). However, further sampling, modeling, and validation at additional field sites with different management practices are recommended to properly confirm CoupModel transportability within the Abbotsford physiographic region.

- In this study, transportable models were found as useful tools to investigate nitrate leaching at various farm-locations within a physiographic region. Some levels of similarity between the investigated locations are required to utilize a transportable model. Required level of similarities can be subjective and different depending on the agricultural and environmental conditions of the landscape for which a transportable model is generated. However, further investigation to set standards for the level of similarity between two sites to facilitate model transportability and quantifying expected error associated with each level is encouraged for broader application of the transportability concept for other case studies.

- Continuation of BMP in Parcel B is necessary in order to observe significant responses, particularly at Station 2 located in Parcel B of the Woodstock Well Field. Also, initiation of BMP at Parcel A is recommended. Particularly, corn under reduced fertilizer application and zero manure supply is recommended in comparison to corn-soybean-winter wheat rotation for more reduction of the nitrate leaching from Parcel A.

- Efficient continuation of field monitoring is necessary in order to support simulation results.

Appendix

Appendix A

Monthly Precipation and Mean Temperature

Monthly precipitation and mean temperature during the growing seasons 1 (March 2009 - October 2009) and 2 (March 2010 - October 2010) and wet/cold seasons 1 (November 2009 - April 2010) and 2 (November 2010 - April 2011) are reflected in Figures A1 and A2.

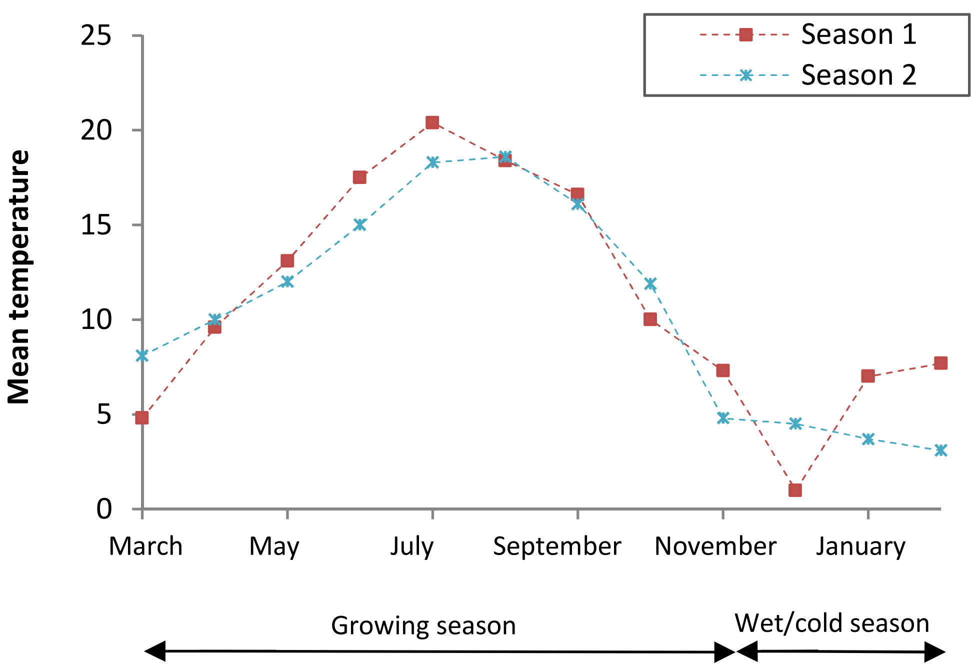

Figure A.1: Monthly precipitation during the study period including two growing seasons (March 2009-October 2010 and March 2010-October 2011) and two wet/cold seasons (November 2009-February 2010 and November 2010-February 2011).

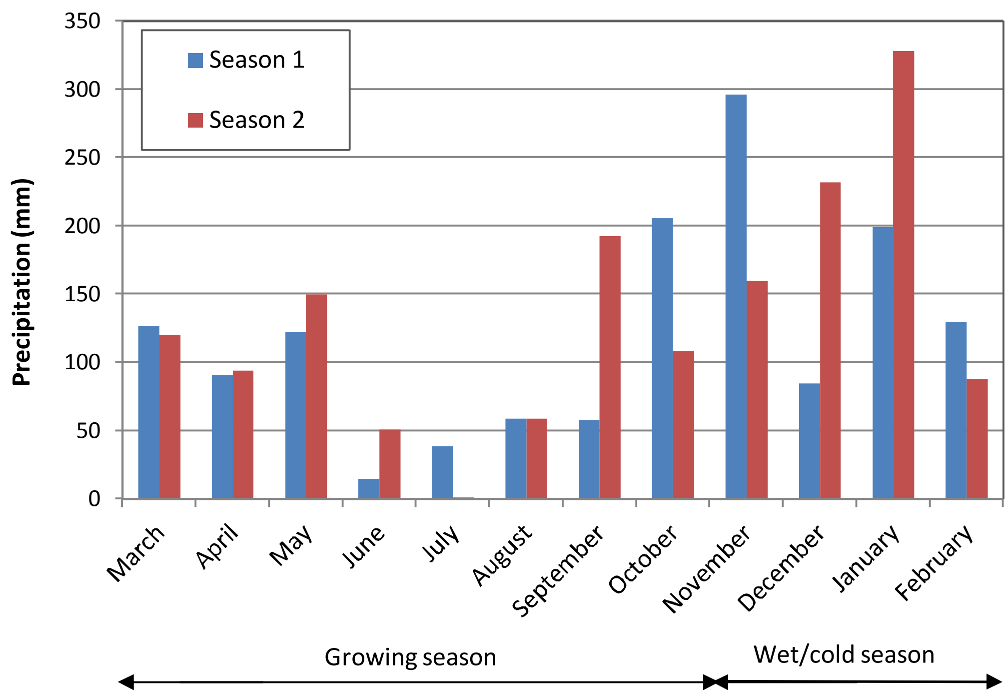

Figure A.2: Monthly mean temperature during the study period including two growing seasons (March 2009-October 2010 and March 2010-October 2011) and two wet/cold seasons (November 2009-February 2010 and November 2010-February 2011).

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