Modeling Subsurface Drainage of Agricultural Fields in High Time Resolution Using RZWQM2

By

Changchi Xian

Department of Bioresource Engineering

Faculty of Agricultural and Environmental Sciences

McGill University

Quebec, Canada

April 2017

A thesis submitted to McGill University in partial fulfillment of the requirements of the degree of Master of Science

Abstract

Mathematical models have been widely used in agricultural fields to simulate hydrologic process and to predict water transport in farmlands. The field-scale Root Zone Water Quality Model (RZWQM version 2.94.00) is proven to be satisfactory in modeling agricultural subsurface drainage in many studies. However, while focusing on long-term period drainage simulation and overall model performance, few study investigates simulations in short-term high drainage peak events, where models usually show relatively unacceptable performance. Alternative methods should be evaluated in improving drainage peak simulations, and high time resolution data should be utilized in these short-term period tests. Therefore, this study aims at: 1) modifying soil water redistribution process in RZWQM2 to solve drainage peak delay issue and improve the simulation in the timing of drainage peak, 2) testing transient state drainage equations (integrated-Hooghoudt Equation and van Schilfgaarde Equation) against the steady state equation (Hooghoudt Equation) on an hourly time scale, 3) evaluating macropore component in RZWQM2 on an hourly scale to test preferential flow effects on drainage peak simulations. Two sets of data collected from subsurface drainage sites were used in this study. One of the experiments was conducted at the Agricultural Drainage Water Quality – Research and Demonstration Site (ADWQ-RDS) in Iowa, USA. And the second experiment was conducted by Agriculture and Agrifood Canada (AAFC) at the north shore of Lake Erie in Harrow, Ontario. The results showed that, by modifying the model to allow soil water redistribution and drainage to occur simultaneously with the infiltration of rainfall, the model performance was significantly better than that in original RZWQM2, with the percent of bias (PBIAS) decreased while Nash-Sutcliffe efficiency (NSE) and Index of Agreement (IoA) increased in both scenarios. However, tile drainage computed using the transient equations didn't improve the model performance. No significant difference amongst those equations was

observed in this study. By activating macropore component in RZWQM2, hourly drainage peak values were better simulated, but it didn't perform satisfactorily in predicting total drainage amount and timing in peak periods. Furthermore, the macroporosity and pore radius parameters in the macropore component were proved to be insensitive. In general, the modified version of RZWQM2 performed better in simulating the timing of hourly drainage peaks and the macropore component can increase simulated peak values which were closer to the observed peak values. More methods should be tested to improve RZWQM2 performance in simulating drainage peak distribution and amount on an hourly time scale.

Résumé

La modélisation mathématique du drainage agricole, largement appliquée sous des conditions rencontrées en champ cultivé, permet de simuler les processus hydrologiques y prévalant et de prédire le mouvement des eaux dans ces terres. Un bon nombre d’études ont démontré l’aptitude du modèle “Root Zone Water Quality Model” (RZWQM version 2.94.00), opérant à l’échelle du champ, à modéliser le drainage agricole souterrain. Mettant plutôt l’accent sur la simulation du drainage à long terme et la performance globale du modèle, rare sont les études s’adressant aux simulations à court terme lors d'événements de débit de pointe, où le modèle montre généralement une piètre performance. Pour ces essais à court terme, des méthodes alternatives pour améliorer la simulation des débits de pointe, incluant l’utilisation de données à une résolution temporelle plus élevée, furent évaluées. L’étude visa à: 1) modifier le processus de redistribution de l’eau à travers le sol opérant dans RZWQM2 afin d’adresser et amenuiser les problèmes de retard et de suite chronologique des débits de pointe simulés, 2) évaluer les équations de drainage en état transitoire (équations intégrées Hooghoudt et van Schilfgaarde) à celle en état d’équilibre (Hooghoudt) à une échelle horaire, et 3) revoir l’élément de RZWQM2 dédié aux macropores afin d’évaluer les effets d’un écoulement préférentiel sur les événements de drainage de pointe simulés à une échelle horaire. La présente étude puisa dans deux ensembles de données de drainage souterrain : une provenant d’une parcelle expérimentale située au Site de recherché et de démonstration sur la qualité des eaux de drainage agricoles de l’université Iowa State (Iowa, É.U.), et une seconde, maintenue par Agriculture et Agroalimentaire Canada, sur la côte nord du Lac Érié, près de Harrow, ON. En modifiant le modèle de manière à permettre une redistribution plus précoce de l’eau dans le sol, de façon que le drainage puisse avoir lieu en même temps que l’infiltration de la pluie, la performance fut améliorée de façon significative par rapport au modèle

RZWQM2 original: le pourcentage de biais diminua, tandis que le coefficient d'efficacité de la modélisation Nash-Sutcliffe et l'indice de concordance (Index of Agreement) augmentèrent pour les deux jeux de données. Cependant, le calcul du drainage souterrain par équations en état transitoire n'améliora pas la performance du modèle, les trois équations ne montrant aucune différence entre elles. Activer l'élément macropore de RZWQM2, permit une simulation plus précise des débits de drainage de pointe à une échelle horaire, mais présenta une piètre performance prédictive quant à la quantité d'eaux de drainage et ses variations temporelles en périodes de pointe. Les résultats de modélisation s'avérèrent peu sensibles aux variations des paramètres de macroporosité et de rayon de l'espace lacunaire de l'élément macropore de RZWQM2. Quoique la version modifiée de RZWQM2 puisse fournir des simulations de drainage de pointe d'une plus grande précision temporelle et, lorsqu'activé l'élément macropore permette une hausse du niveau des événements de drainage de pointe simulés, s'approchant ainsi plus près des niveaux de pointe observés. On se doit d'évaluer des méthodes supplémentaires pour améliorer la performance de RZWQM2 quant aux variations temporelles et quantités absolues lors d'événements de drainage de pointe simulés à une échelle horaire.

Acknowledgements

I would like to thank my supervisor Dr. Zhiming Qi for his constant guidance and support in my research, as well as his patience and understanding throughout my graduate study in McGill. I would also express my great appreciation to my committee member Dr. Shiv Prasher for his kindness in helping me to solve problems in my study and offering detailed instructions.

I would like to thank Dr. Liwang Ma and Dr. Lajpat R. Ahuja for providing the codes of RZWQM2 software, and helping me to review my work. I would also like to thank Dr. Chin S. Tan and Dr. Tiequan Zhang from Agriculture and Agri-Food Canada in Harrow, Ontario for generously providing valuable field data which is essential for completing my work. I sincerely appreciate Dr. Georges T Dodds for helping me with the French in my abstract and improving language in my full thesis.

Meanwhile, I would like to thank all my friends and my fellow graduate students for their friendship and support in everyday of my graduate life. Finally I thank my family for their unconditional support and encouragement during these years.

Thank you!

Preface and Contribution of Authors

This thesis contains cover page, abstracts in both English and French, acknowledgement, table of contents, list of tables, list of figures, major content, and references. The major content includes four chapters, respectively, Chapter 1: Introduction; Chapter 2: Modeling hourly subsurface drainage using steady-state and transient methods; Chapter 3: Testing Macropore Component of RZWQM2 in Subsurface Drainage Peak Simulation on Hourly Time Scale; and Chapter 4: Summary and Conclusion. There are connecting statements before Chapter 2 and Chapter 3.

This thesis aims at improving RZWQM2 performance in simulating subsurface drainage on a high time resolution hourly scale. Chapter 2 is a study attempting different assumptions and drainage equations in the model; the manuscript is prepared to be published in Journal of Hydrology. Chapter 3 is another study evaluating effectiveness of macropore component on hourly drainage simulation; the manuscript is also expected to be published in the relevant journal in the future. The manuscripts are co-authored by my supervisor Dr. Zhiming Qi, and also Dr. Tie-Quan Zhang, Dr. Chin S. Tan, and Dr. Liwang Ma.

Table of Contents

List of Tables

List of Figures

Chapter 1. Introduction

1.1 General introduction

Subsurface drainage is an important and widely used approach in water table management, which helps to control soil water content and water table depth in farmland, and aims at improving crop yield and increasing profit. By discharging excess water from precipitation, adjusting fluctuated water table and increasing percolation (Baker *et al.*, 1976), it prevents the crop roots from oxygen deficiency and bad growth, also, it solves the problems of waterlogging and soil salinity. Many researches have shown the evident positive effect of subsurface drainage on crop yield. A 5 years research in a waterlogged saline area also indicated the drained field yield increase in different crops, ranging from 18.8% to 27.6%, and a 35.7% decrease in soil salt contain, compared with the non-drained field (Sharma *and* Gupta, 2005). Comparing controlled drainage with free drainage systems, another study in Ohio, United States tested the crop yield in controlled-drained field and free-drained yield, indicating that the production of corn, popcorn and soybean increased significantly with 3.3%, 3.1% and 2.1%, respectively (Ghane *et al.*, 2012).

Meanwhile, subsurface drainage is a main source of nutrient loss (nitrate-nitrogen, phosphorus, etc.) from farmland, which may also account for pollution in groundwater and surface water bodies since the discharged water with high concentration of N, P and pesticide will lead to eutrophication and water quality degradation. A work in south-central Minnesota reduced 20% drainage volume by changing drainage depth and intensity, demonstrated an 18% reduction of nitrate load in tile flow water (Sands *et al.*, 2007). As well as in Iowa, the nitrogen loss significantly increased in main subsurface drainage period (Baker *et al.*, 1975; Cambardella *et al.*, 1999), which indicated that the nutrient loss is highly related to drainage. A study in southwestern Ontario, Canada, showed the installation of subsurface drainage tile enhances non-point source pollution, especially in heavy rainfall season and non-growing season, when the volume of tile flow out water was higher (Liu *et al.*, 2011). Similar situation occurred in the Mississippi River, whose nitrate loads resulted in a hypoxic zone in the Gulf of Mexico (Rabalais *et al.*, 2001).

Thus, a better understanding of subsurface drainage is essential to controlling quantity and quality of water in agricultural lands, and assessing field condition and developing proper management practices. Agricultural model is a more efficient way to interpret the processes and interactions of an agricultural system, compared with the conventional way by field experiment which is limited by crops life circle and unexpected climatic conditions and usually -time consuming. With the development of computer technology and agricultural science, using computer models to simulate agricultural processes can definitely shorten the time circle in work and also provide a relatively accurate result.

Hydrologic component is one of the basic modules in many agricultural models, such as RZWQM2, DRAINMOD, SWAT, GLEAMS, etc. The main processes including infiltration, evapotranspiration, water table fluctuation and subsurface drainage are simulated based on different theories and assumptions in those agricultural models. Many studies were conducted to evaluate the performance of agricultural models (RZWQM 1999; Skaggs, 1978; Z. Qi *et al.*, 2015; Valentina Krysanova *and* Mike White 2015; Skaggs, 1982). They indicated that these models can provide satisfactory performance in subsurface drainage simulation.

Root Zone Water Quality Model (RZWQM version 2.94.00) is a comprehensive 1-D field-scale agricultural model which was firstly established in 1992, and have been developed and integrated with other models afterward. It is used in modelling the interactions among hydrology, agricultural management, crop growth and chemical fate in farmlands (RZWQM 1999). The subsurface drainage component was added into RZWQM2 in 1994, to enable this model to simulate drain flow in soils have subsurface drainage (P. Singh *and* R. S. Kanwar 1994).

The performance of the hydrologic component had been tested in many studies (Kanwar *et al.*, 1993; Qi *et al.*, 2011) and was proven to be satisfactory in subsurface drainage simulations. However, some approaches could be applied to improve model performance. Most of the studies were focusing on annual and daily overall drainage simulation, while drainage events usually occur in some intensive seasons during a year, and most of the drainage peaks which contribute large fraction of annual total amount only occur in a few days. Therefore, it would be more effective to demonstrate drainage process by investigating the short-term drainage peaks instead of overall simulation, and higher time resolution data should be applied to evaluate model performance in precise time steps. In addition, RZWQM2 uses a steady state drainage equation to compute drainage rate, assuming the outflow water is equal to recharge water from rainfall and irrigation during the drainage period. Other alternative transient state equations (Oosterbaan, 1994), which assume water table keeps fluctuating during drainage, are seldom used in agricultural models although they seem to be closer to reality. Furthermore, the macropore component in RZWQM2 is rarely activated in drainage simulation scenarios. However, the macropores created by crop plants' roots and tillage practice should be considered, and the preferential flow also affects drainage timing and peaks (Beven *and* Germann, 1982; Beven *and* Germann 2013).

1.2 Objectives

This study is the first time using hourly time scale data to evaluate hydrologic component of RZWQM2. By focusing on short-term drainage peak periods, we tested different approaches to improve model performance in drainage peak simulations. The objectives include:

1) Modifying soil water redistribution process in RZWQM2 to solve drainage peak delay issue and improve peak timing simulations.

2) Testing transient state drainage equations (integrated-Hooghoudt Equation and van Schilfgaarde Equation) against the steady state equation (Hooghoudt Equation) in hourly time scale.

3) Evaluating macropore component in RZWQM2 on an hourly scale to test preferential flow effects on drainage peak simulations.

Connecting Statement to Chapter 2

In Chapter 2, RZWQM2 was modified with a new rainfall infiltration assumption, meanwhile two transient state drainage equations were evaluated in both the original and modified RZWQM2, based on hourly observed data from Iowa and Ontario. This study aims at improving RZWQM2 performance in short time scale by using different assumptions and equations.

Chapter 2 is a manuscript prepared for publishing in Journal of Hydrology. The manuscript is co-authored by my supervisor Dr. Zhiming Qi, and also Dr. Chin S. Tan, Dr. Tiequan Zhang.

Chapter 2. Modeling Hourly Subsurface Drainage Using Steady-state and Transient Methods

2.1 Abstract

Computer models have been frequently used to simulate the hydrologic and environmental processes in subsurface-drained cropland. The widely-tested steady-state Hooghoudt (*ssH*) equation, implemented in the Root Zone Water Quality Model (version 2.94.00), serves in simulating subsurface drainage. However, transient methods such as the integrated Hooghoudt (*inH*) and van Schilfgaarde (*vanS*) equations have seldom been implemented in models. In the present study, RZWQM2's hydrologic component was modified to initiate the soil water redistribution process when rainfall occurred. The three drainage equations (*ssH*, *inH* and *vanS*) were tested in each of two versions of RZWQM2 (original and modified). Field data from Iowa (2007-2008) and Ontario (2009-2010) were used to evaluate different model version × equation combinations' simulation accuracy at both daily and hourly scales, evaluated using the percent of bias (*PBIAS*), Nash-Sutcliffe efficiency coefficient (*NSE*), and the Index of Agreement (*IoA*). On a daily scale and across equations, for the Iowa data the original model ($PBIAS \leq 14.96$, $NSE \geq 0.40$, $IoA \geq 0.69$) was outperformed by the modified model ($PBIAS \leq 6.48$, $NSE \geq 0.70$, $IoA \geq 0.76$). Similarly, for the Ontario data, the original model ($PBIAS \leq 8.87$, $NSE \geq 0.19$, $IoA \geq 0.65$) was outperformed by the modified model ($PBIAS \leq 3.59$, $NSE \geq 0.31$, $IoA \geq 0.67$). However, based on a parity of *PBIAS*, *NSE* and *IoA* values, hourly scale tile drainage computed using the modified model equipped with transient equations did not improve model performance compared with the original *ssH* equation.

Keywords: RZWQM2, model development, subsurface drainage equation

2.2 Introduction

As an important physical component in agricultural systems, subsurface drainage is implemented to improve crop yield and increase profits. Tied to factors such as drain layout, weather, soil texture and irrigation rates and methods, tile drainage flow rates from agricultural lands influence water table levels as well as with nutrient and pesticide losses to groundwater (Stämpfli *and* Madramootoo, 2006; Baker *and* Johnson, 1981). The development of computer technology and agricultural science has provided the capacity to accurately simulate agricultural processes rather than to resort to time- and cost-inefficient field experimentation. Generally used in simulating cropping systems and predicting the effects of different agronomic operations, such soil-water-crop-climate system models (*e.g.* RZWQM2, DRAINMOD, SWAT, GLEAMS) almost invariably include a hydrologic module. Such models have been shown to provide acceptable simulations of subsurface drainage flow (Qi *et al.*, 2011; Ma *et al.*, 2007; Wang et a*l.*, 2005; Singh *et al.*, 2006; Moriasi *et al.*, 2013; Gowda *et al.*, 2012; Sogbedji *and* McIsaac, 2002; Ritzema *et al.*, 2007; Sharma *and* Gupta, 2005).

The Root Zone Water Quality Model (version 2.94.00) is a widely-used agricultural system model first developed in 1992, and subsequently coupled with other models such as DSSAT and SHAW. Compared with other models, RZWQM2 provides a more comprehensive simulation of agricultural systems, including the interactions between hydrology, agricultural management, crop growth and chemical fate in farmlands (Ahuja *et al.*, 2000). A subsurface drainage component was incorporated into RZWQM2 in 1994, enabling the model to simulate tile drainage flow (Singh *and* Kanwar, 1994). This hydrologic component is the core of RZWQM2, which coordinates with other components in modeling crop, chemicals transportations and management practice. Therefore, improving subsurface drainage simulation in RZWQM2 can lead to robust model performance in other related functionalities.

The performance of RZWQM2's hydrologic component was tested on different scenarios of subsurface drain flow data, and the overall performance was deemed acceptable (Kanwar *et al.*, 1997; Akhand *et al.*, 2003.). Simulations of hydrologic process occurring under a corn-soybean rotation operating under different land cover treatments in north central Iowa, found simulated annual cumulated subsurface drainage volume to closely match observed data: the percent of bias (*PBIAS*) being within 11% for calibration plots, and within 5% for validation plots. For both plots the Nash Sutcliffe Efficiency coefficient (*NSE*) exceeded 0.84, and the ratio of the root mean square error to the standard deviation (*RSR*) was below 0.40 (Qi *et al.*, 2011). However, some delays in simulated (vs. actual) drainage were observed for extended rainfall events in this study, and the high drainage peaks were underestimated in this scenario. These problematic simulations may due to inadequate methods of subsurface drainage calculation in RZWQM2, and alternative approaches should be tested to improve the model.

In the original RZWQM2, the onset of a rainfall or irrigation event would activate the simulation of infiltration processes using the Green-Ampt model. As Richards' equation is not applied to the redistribution of soil moisture in the profile during infiltration, infiltrated water is held above the wetting front. It is not distributed to the unsaturated soil profile below the wetting front and not used to raise the water table until the rainfall ceases. A constant drainage rate which begins when rain starts and is calculated using a constant water table height above the drain, along with unit gradient flow in an unsaturated soil matrix are used to accumulate drain outflow over this period (Ahuja L *et al.*, 2000). At the onset of the current infiltration event this outflow is calculated using the steady-state Hooghoudt (*ssH*) equation. During infiltration this constant drainage rate will be updated only if the wetting front reaches the water table, resulting in ponding conditions. For extended rainfall events, which usually also coincides the periods of elevated drainage, drainage would occur with a delay of at most one day. This delay could be critical for agricultural contaminants modeling, as many pesticides and herbicides have short degradation half-lives, and the fate and subsurface transport of these contaminants are highly related to subsurface drainage (Malone *et al.*, 2004). The high concentration of the contaminants in the leachate is usually accompanied by intensive drainage (Kumar *et al.*, 1998). Therefore, higher accuracy in drainage peak simulations also benefits the prediction in the fate of agricultural contaminant. To simulate soil water movement more appropriately and solve the drainage delay problem, rainfall and redistribution of water in the soil profile must be assumed to occur simultaneously.

In addition, the appropriateness of using the *ssH* drainage equation to compute subsurface drainage has been questioned in a number of studies which attempted to identify alternative drainage equations offering better simulation accuracy (Shokri *and* Bardsley, 2014; Mishra *and* Singh, 2010; Pali *et al.*, 2014). Drainage equations can be classified into two principal categories: steady-state equations and non-steady-state (transient) equations (Oosterbaan, 1994). Steady-state equations, rather quasi-steady state equations, assume that drainage outflow is equal to the net recharge over a given period of time, with the water table remaining at the same depth during this period (Darzi-Naftchally *et al.*, 2014), but changing between the time periods. Common steady-state equations include the Hooghoudt, Kirkham, Ernst, and Dagan equations. Comparatively, in the case of transient equations recharge and discharge differ: (i) when recharge exceeds discharge, the water table rises, resulting in a rise in discharge rate until it reaches the inflow rate, (ii) when discharge exceeds recharge, both the water table and drainage rate drop. As a result, under transient conditions the water table fluctuates around an average depth during a given period.

The objectives of this study were therefore to: 1) the first time to modify RZWQM2's hydrologic component and improve drainage flow simulation by allowing soil moisture redistribution and drainage to occur simultaneously with rainfall, and 2) to compare the accuracy in simulating daily and hourly tile drainage of the transient *inH* and *vanS* equations to that of the standard *ssH* equation. The comparisons in this study are based on precise hourly data which is seldom used in drainage simulation. Hourly data can be used to more precisely evaluate the accuracy of a model (Kohler *et al.*, 2001), since a peak drainage event usually last for only a few hours. The subsurface drainage hydrograph on a daily scale are vague, while hourly hydrograph can provide much more detailed information about the timing of drainage peaks.

2.3 Materials and Methods

2.3.1 Modification of the approach in simulating tile drainage

In order to solve the delayed drainage peaks due to inappropriate soil water redistribution method in the original RZWQM2, we modify the model to represent the situation observed in experimental plots. Redistribution of water in the soil profile and subsurface drainage are assumed to occur simultaneously with rainfall. To achieve this modification, we reset the starting time step of soil water redistribution as the first time step of the rainfall event. During the rainfall, the constant drainage rate will be replaced with a dynamic drainage rate computed using *ssH* and changing water table (the modifications to the RZWQM2 code are provided in Appendix). Drainage flow data during 2007 and 2008 from Iowa, and during 2009 and 2010 from Ontario were used to evaluate the accuracy of simulations. Information regarding measured data is presented in the Observed data and parameterization section.

2.3.2 Different equations to simulate tile drainage

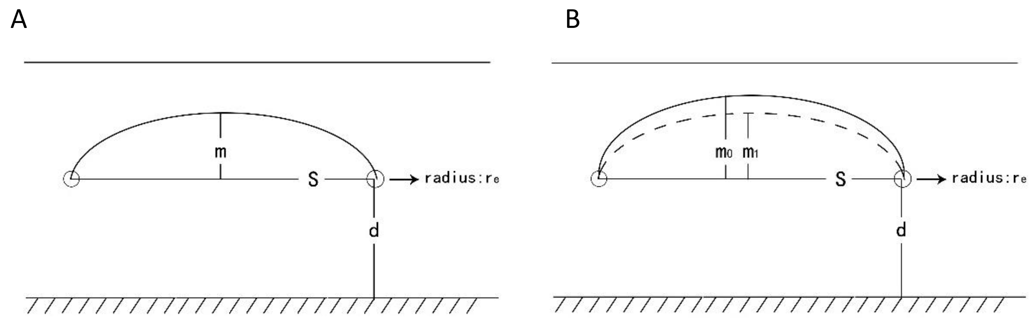

Figure 1. Steady state (A) and transient (B) drainage systems: m, m_0 and m_1, depth from the midway-between-drains water table to the drains in steady state, before and after drainage respectively (m); d, actual depth of the soil profile (m); r_e, radius of the drains (m); and S, drain spacing (m).

In RZWQM2's basic hydrology module the steady state Hooghoudt equation (*ssH*) is used to calculate the subsurface drainage rate *R* (USDA-ARS. 1992). This equation assumes that the water table is unchanged during the drainage period (Fig 1A):

$$R = \frac{8K_e d_e m + 4K_e m^2}{S^2} \quad (1)$$

where,

m	is the depth from the midway water table to the drains (m)
d_e	is the effective depth of the soil profile (m)
K_e	is the effective hydraulic conductivity (mm h^{-1}), and
S	is the drain spacing (m)

The value of K_e is calculated as (USDA-ARS. 1992):

$$K_e = \frac{\sum_{i=1}^{i=n} D_i K_i}{\sum_{i=1}^{i=n} D_i} \quad (2)$$

where,

n is the number of soil layers (set by model user),

D_i is the thickness of layer I (m), and

K_i is the lateral hydraulic conductivity of layer i (mm h^{-1})

The value of d_e is calculated differently according the actual depth of the soil profile:

$$\text{if } \frac{d}{S} < 0.3 \qquad d_e = \frac{d}{1 + \frac{d}{S}\left[\left(\frac{8}{\pi}\ln\frac{d}{r_e}\right) - CON\right]} \tag{3}$$

$$\text{where, } \qquad CON = 3.55 - 1.6\frac{d}{S} + 2\left(\frac{d}{S}\right)^2 \tag{4}$$

$$\text{or, if } \frac{d}{S} \geq 0.3 \qquad d_e = \frac{S}{\left(\frac{8}{\pi}\ln\frac{S}{r_e}\right) - 1.15} \tag{5}$$

where,

d is the actual depth of the soil profile (m), and

r_e is the radius of drains (Fig. 1).

In contrast, in using the van Schilfgaarde (Bouwer *and* van Schilfgaarde, 1963) transient state equation (*vanS*) to calculate drainage, the difference in water table height before and after a specific time period is taken into account (Fig. 1B):

$$S = 3A\sqrt{\left[\frac{K_e(d_e + m)(d_e + m_0)t}{2f(m_0 - m)}\right]} \tag{6}$$

$$\text{where, } \qquad A = \sqrt{\left[1 - \left(\frac{d_e}{d_e + m_0}\right)^2\right]} \tag{7}$$

where,

m and m_0 are the midway water table heights (relative to the drain) after and before drainage, respectively (Fig. 1B)

f is drainable porosity (mm^3 mm^{-3})

t is the time period (h)

For a known drain spacing and initial water table height, Eq. 6 can be used to calculate the change in water table height (ΔH) from before (m_0) to after drainage flow (m) (Figure 1B):

$$m = \frac{Mm_0 - Nd_e}{M + N} \tag{8}$$

where, $M = 2fS^2(d_e + m_0)$ (9)

and $N = 9K_e t m_0(2d_e + m_0)$ (10)

To circumvent the shortcomings of Eq. (6) under large time increments, Bouwer and van Schilfgaarde (1964) developed a solution to the van Schilfgaarde (1963) equation, which is derived from a mass balance coupled with a steady state Hooghoudt equation, namely the integrated Hooghoudt equation (*inH*) used in this study:

$$S = \sqrt{\frac{9K_e t d_e}{f\ \ln\left(\frac{m_0(2d_e + m)}{m(2d_e + m_0)}\right)}} \tag{11}$$

In order to calculate drainage flow, Eq. 12 is altered to provide the final water table height:

$$m = \frac{2d_e m_0}{2d_e e^Z + m_0 e^Z - m_0} \tag{12}$$

where, $Z = \frac{9Ktd_e}{fS^2}$ (13)

The product of ΔH (*i.e.* $m_0 - m$) by *f* yields the drainage coefficient (*DC*) and thereby the drain out flow:

$$DC = f * \Delta H \tag{14}$$

For a specific soil profile, the drainable porosity is calculated as (Ma *et al.*, 2007):

$$f = \theta_{sat} - \theta_{fc} \tag{15}$$

where,

θ_{fc} is the soil moisture at field capacity (mm^3 mm^{-3}), *i.e.* at a soil matric potential $\psi_m = -33$ kPa, and

θ_{sat} is the soil moisture at saturation (mm^3 mm^{-3}), *i.e.*, at $\psi_m = 0$ kPa.

As RZWQM2 uses very small time steps (≤0.1 hour) in each iteration of hydrologic process and soil water update, the shortage of *vanS* in large time increments is avoided. Therefore, both of the two transient equations (*vanS* and *inH*) are tested in this study. To test the two transient equations against the steady state equation, the source code of RZWQM2 was modified. In RZWQM2, soil water redistribution is determined by the Richards equation, after each time step of model calculations, the soil water content in every node of the soil matrix is updated based on the numerical solution of a 1-D Richards equation, and then the water table is also updated according to the new soil water distribution. In the original model, the *ssH* equation obtains current water table height from the model, computes drainage rate by Eq. 1, and returns the value to model. After the drainage process, water table is updated again according to the calculated drainage rate, the updated water table will be the initial water table height in the next time step calculation. With the modifications of equation, we still obtain initial water table height from the model, *inH* (Eq. 8) and *vanS* (Eq. 12) are used to compute an estimated new water table m, then our drainage rate is determined by Eq. 14, and this result will be returned to the model for the following calculations and processing to next time steps.

2.3.3 Observed data and parameterization

Two sets of data were used to assess different modifications of RZWQM2 in this study. The first field study was conducted at the Agricultural Drainage Water Quality – Research and Demonstration Site (ADWQ-RDS) near Gilmore City in Pocahontas County, north central Iowa. The second experiment was conducted by Tan *et al.* (2009), on an experiment field located at the north shore of Lake Erie in Harrow, Ontario.

Iowa experiment

The experiment near Gilmore City, Iowa started in the fall of 2004 and continued for five years, with a complete randomized block design of 78 individually-drained plots. The size of each plot was 38 m in length and 15.2 m in width and total research area is 4.5 ha. The field is in a flat area with average slope of 0.5–1.5% (Lawlor *et al.*, 2008; Qi *et al.*, 2008; Singh *et al.*, 2006). The plots were established after the installation of corrugated plastic drain lines through the center and both boundaries parallel to the long dimension (7.6 m drain spacing) at a depth of 1.06 m. In the present study, data was collected between 2007 and 2008 from four plots with a corn (odd year)-soybean (even year) rotation on an hourly scale. Winter wheat served as a cover crop prior to main crop planting in each year. Hourly drainage from each plot was observed during the experimental period. Drainage flow volume for each plot was measured using a magnetic flow meter connected to an electronic data logger; meter readings were also recorded manually (Qi *et al.*, 2008). Since there is a high field variability in tile drainage amount amongst the plots, all the plots were blocked into 4 drainage groups: high, medium high, medium low and low. For each treatment, four plots, one from each block, were randomly selected and assigned. The average of the measured flow rate over 4 plots was used as observed hourly drainage data in this study.

All the parameters employed to set up scenarios in the present study were previously calibrated (Qi *et al.*, 2011) (Table 1). Predominant soils in the field were Nicollet (fine-loamy, mixed, superactive, mesic Aquic Hapludoll) and Webster and Canisteo (fine-loamy, mixed, superactive, mesic Typic Endoaquolls) clay loams. Soil cores were extracted from the following depths: 50-150, 150-250, 250-350, 350-450 and 550-650 mm for each sampling location, which was 1 meter apart from each other along the midway between the center and boundary lines. Soil hydraulic properties, bulk density, particle size distribution, saturated hydraulic conductivity and soil water characteristic curves were determined from undisturbed soil cores. Lateral hydraulics conductivities (K_{sat}^{lat}) in each layer were adjusted to $2K_{sat}^{\mathrm{ver}}$, in order to match the peaks of daily drain flow. Bubbling pressure and pore size distribution were fit using the Brooks-Corey equation. Residual water content, soil moisture at different matrix potentials (-10, -33 and -1500 kPa) were interpolated or extrapolated from the soil water characteristic curve. During the five-year experiment period, hourly meteorological data including rainfall, air temperature, solar radiation, relative humidity and wind speed were collected by an automatic meteorological station installed at the site. Greater details of the experiment design and data collection can be found in Helmers *et al.* (2005) and Singh *et al.* (2006).

Table 1. Calibrated soil hydraulic properties in Iowa

Depth (m)	ρ (Mg m^{-3})	*Sand* (g g^{-1})	*Silt* (g g^{-1})	K_{sat}^{ver} (mm h^{-1})	K_{sat}^{lat} (mm h^{-1})	Soil moisture content, θ (mm^3/mm^3) Soil matric potential, ψ_m (kPa)				
						θ_{sat} 0 kPa	θ_{10} -10kPa	θ_{fc} -33 kPa	θ_{pwp} -1500kPa	θ_{r} -∞ kPa
0-0.10	1.37	0.32	0.36	48	97	0.482	0.383	0.376	0.1887	0.0705
0.10-0.20	1.38	0.32	0.36	33	66	0.476	0.384	0.376	0.2304	0.0718
0.20-0.30	1.39	0.33	0.53	51	101	0.473	0.384	0.376	0.2005	0.0787
0.30-0.40	1.39	0.40	0.30	40.8	82	0.474	0.384	0.399	0.2115	0.0721
0.40-0.60	1.39	0.46	0.30	40.8	82	0.474	0.408	0.368	0.2178	0.0645
0.60-0.90	1.45	0.44	0.34	26.4	53	0.450	0.380	0.368	0.2038	0.0339
0.90-1.20	1.46	0.44	0.34	26.4	53	0.450	0.312	0.299	0.1844	0.0325
1.20-2.00	1.46	0.44	0.34	26.4	53	0.450	0.310	0.299	0.1678	0.0325
2.00-3.00	1.5	0.44	0.34	26.4	53	0.450	0.310	0.299	0.1678	0.0325
3.00-3.90	1.5	0.44	0.34	0.001	50	0.450	0.310	0.299	0.1678	0.0325

Note: ρ = soil bulk density; *Sand (50–2000 μm) and Silt (2–50 μm) fractions;* K_{sat}^{ver} *and* K_{sat}^{lat}, *vertical and lateral saturated hydraulic conductivity, respectively.*

Three periods of at least 5 days, each bearing a single drainage peak, were selected in 2007 and 2008: (i) 24-28 May, 2007, (ii) 19-25 August 2007, and (iii) 18-22 October 2007. These periods' relatively taller drainage peaks allowed a better assessment of whether simulations matched observed drainage data, and were therefore deemed more reliable and representative in evaluating the performance of different drainage equations at an hourly scale, particularly in peak drainage periods.

Ontario experiment

The experiment in Harrow, Ontario was started in the spring of 2008, on a site consisting of 16 drained plots (Tan *et al*., 2009). Every plot was 131×25 m designed in the flat field, with buffer zones and impermeable barriers installed to prevent interaction amongst plots. In the present study, 2009 to 2010 data from two plots in the larger experimental field served to test different hydrologic simulations in RZWQM2. Two 104-mm diameter subsurface tile drains were installed parallel along the length of the plot at 0.6 m depth and 4.6 m spacing with a less than 0.1% slope. For each plot, a tipping bucket was used to automatically measure tile drainage volume on a continuous year-round base. A magnetic reed switch was mounted on each bucket, so that every tip produced a switch closure detected by a multi-channel data logger. The data logger counted these signals and converted them to flow volume on a continuous base. The average observed values from the two plots served as the calibrated observed drainage flow in this study due to variability existed in plots.

The predominant soil in these fields was a Brookston clay loam, with an average of 28% sand, 37% silt and 35% clay, a mean measured bulk density of 1.34 mg m^{-3}, a measured soil porosity of 52.4% and a measured saturated hydraulic conductivity ranging from 17 to 119 mm day^{-1}, with an average K_{sat}^{ver} of 50 mm day^{-1} (Liu *et al*., 2011). Lu (2015) calibrated the RZWQM2 against measured data from this Ontario site. Lateral hydraulic conductivity (K_{sat}^{lat}) was adjusted to be equal to saturated conductivity (K_{sat}^{ver}) in each soil horizon. The bubbling pressure was calibrated against the observed drainage flow, and the saturated soil water content was assumed equal to the measured soil porosity. In the scenario from Lu (2015), drainage simulation in the winter period was not satisfactory. Accordingly, observed data from a non-freezing period (i.e. April to October) in 2009 and 2010 were used in this study. Hydraulic parameters were recalibrated to match hourly observations, based on a scenario from Lu (2015) (Table 2).

Hourly weather data including rainfall, air temperature, solar radiation, wind speed and relative humidity were recorded during the whole study period at the local weather station in Whelan, ON, located less than 0.5 km from the experiment site. However, the rainfall measurements between Jan 1st 2009 and April 30th 2009 were incorrect due to measurement problems. Therefore, rainfall data used for this period were from the Harrow weather station located 16.6 km away from the site. More explicit information of experiment design and data collection can be found in Tan *and* Zhang (2011).

For drainage equations comparisons, we again selected three peak periods to allow an hourly scale assessment, including: (i) 4-8 April 2009, (ii) 18-22 April 2009, and (iii) 4-8 June 2010.

Table 2. Calibrated soil hydraulic properties in Ontario

Depth (m)	ρ (Mg m^{-3})	Sand (g g^{-1})	Silt (g g^{-1})	K_{sat}^{ver} (mm h^{-1})	K_{sat}^{lat} (mm h^{-1})	Soil moisture content, θ (mm^3 mm^{-3}) Soil matric potential, ψ_m (kPa)				
						θ_{sat} 0 kPa	θ_{10} -10kPa	θ_{fc} -33 kPa	θ_{pwp} -1500kPa	θ_r -∞ kPa
0-0.25	1.326	0.299	0.363	9.2	17	0.5	0.383	0.325	0.1983	0.04
0.24-0.45	1.391	0.238	0.349	38	68	0.475	0.378	0.336	0.2395	0.09
0.45-0.80	1.391	0.257	0.33	30	60	0.475	0.371	0.330	0.2356	0.09
0.80-1.20	1.391	0.243	0.359	20	40	0.475	0.390	0.347	0.24576	0.09
1.20-3.00	1.391	0.243	0.359	5	20	0.475	0.390	0.347	0.24576	0.09
3.00-3.09	1.391	0.243	0.359	0.1	20	0.475	0.390	0.347	0.24576	0.09

Note: ρ = soil bulk density; *Sand (50–2000 µm) and Silt (2–50 µm) fractions;* K_{sat}^{ver} *and* K_{sat}^{lat}, *vertical and lateral saturated hydraulic conductivity, respectively*.

2.3.4 Testing different versions of RZWQM2

Two approaches to subsurface drainage simulation were tested: the original scenario of the drainage rate being maintained throughout rainfall ($RZWQM2_0$), and a scenario where soil moisture was redistributed during rainfall ($RZWQM2_R$). These were factorially combined with three drainage equations (*ssH*, *inH* and *vanS*), resulting in 6 RZWQM2 runs for each of the two sets (Iowa, Ontario) of data:

$$RZWQM2_0^{ssH}, RZWQM2_0^{inH}, RZWQM2_0^{vanS}, RZWQM2_R^{ssH}, RZWQM2_R^{inH}, RZWQM2_R^{vanS}$$

2.3.5 Statistical methods for model accuracy evaluation

To evaluate the performance of these equations, the percent of bias (*PBIAS*), Nash-Sutcliffe efficiency coefficient (*NSE*) and Index of Agreement (*IoA*) were used to assess how well model drain flow outputs matched measured drain flow:

$$PBIAS = 100 \cdot \frac{\sum_{i=1}^{n}(S_i - O_i)}{\sum_{i=1}^{n} O_i} \quad (16)$$

$$NSE = 1 - \frac{\sum_{i=1}^{n}(O_i - S_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \quad (17)$$

$$IoA = 1 - \frac{\sum_{i=1}^{n}|S_i - O_i|}{2\sum_{i=1}^{n}|O_i - \bar{O}|} \quad (18)$$

where,

n is the number of measured (and simulated) values,

O_i is the i^{th} observed value,

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

S_i is the i^{th} simulated value.

In the drainage flow simulation, *PBIAS* within ±15%, *NSE*>0.70, and *IoA* close to 1 indicate a satisfactory model performance for a daily time step using RZWQM2 (Moriasi *et al.*, 2015). These criteria are only used to evaluate model modifications on daily time scale. However, for the hourly scale comparisons, there is no available criterion, so we compared the differences in *PBIAS*, *NSE* and *IoA* between modeling methods.

2.4 Results and Discussion

2.4.1 RZWQM2$_R$ *vs.* RZWQM2$_O$

Unlike the original $RZWQM2_0$ model, the $RZWQM2_R$ model allows soil moisture redistribution and tile drainage to happen simultaneously with the rainfall, thereby adapting it to extended rainfall conditions, and avoiding drainage peak delays after infiltration occurs. Figure 2 shows a typical drainage peak period in Iowa scenario, providing insight as to how the modifications alter simulated results on an hourly basis under intensive rainfall conditions. Instead of holding infiltrated water above wetting front, $RZWQM2_R$ starts soil water redistribution when rain starts, and calculates drainage rate using a dynamic water table height; therefore, it avoids obvious delays in peak occurrence under long-term rainfall, and improves model performance. The effects of this modification on other hourly drainage peaks were similar in both Iowa and Ontario scenarios, there being improvements in hourly drainage simulation accuracy. Accordingly, the two versions of the model were evaluated at the daily scale.

Comparing both $RZWQM2_0$ and $RZWQM2_R$ simulations to daily drainage flow data from Iowa for 2007 and 2008 (Figures 3A, 3B, respectively), as well as model accuracy statistics (Table 3) show $RZWQM2_R$ to have perform significantly better in simulating subsurface drainage patterns than $RZWQM2_0$. The predicted cumulative drainage volume over a two-year period

(2007 and 2008) simulated by $RZWQM2_0$-ssH and $RZWQM2_R$-ssH were 920.9 mm and 862.8 mm respectively, compared to an observed total of 810.4 mm.

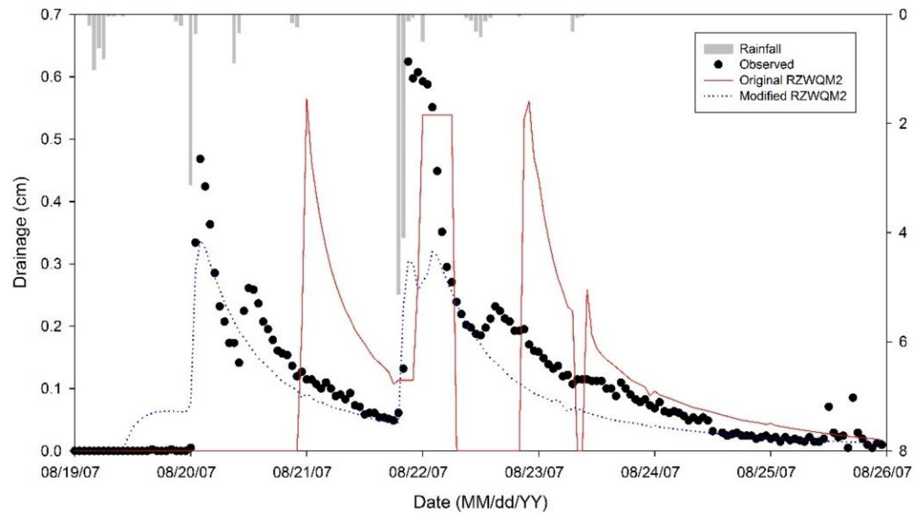

Figure 2. Observed hourly drainage and hourly drainage simulated by original and modified versions of RZWQM2 ($RZWQM2_0$ and $RZWQM2_R$) using the default Hooghoudt Equation (ssH): 19-25 August 2007, Iowa.

The $RZWQM2_0$-ssH and $RZWQM2_R$-ssH models' simulation of daily drainage flow over a 2-year period were compared. Changing from the $RZWQM2_0$-ssH to the $RZWQM2_R$-ssH model resulted in an improvement of *PBIAS*, *NSE*, and *IoA* (Table 3). The $RZWQM2_R$ model performed significantly better than the $RZWQM2_0$ not only for the *ssH* equation, but also with the *inH* and *vanS* transient equations, with the *NSE* increasing from 0.41 and 0.70, and the *IoA* rising from to 0.70 and 0.76 in both cases. For the $RZWQM2_R$ model, only minor differences in simulated drainage volume and timing were apparent across the three equations (*ssH*, *inH*, and *vanS*), with simulated values of 862.8, 862.3 and 862.4 mm (Table 3). The *NSE* and *IoA* for the *inH* and *vanS* equations were same for both models (0.70 and 0.76, respectively), and largely the same as those for the *ssH* equation (0.71 and 0.76, respectively). The similar lack of differences in simulated drain flow among the different drainage equations was apparent for the $RZWQM2_0$ model (Table 3). Overall the $RZWQM2_R$ model was more accurate than the $RZWQM2_0$ model in predicting daily drainage flow under heavy rainfall conditions, but the type of equation used to calculate drainage flow had little effect.

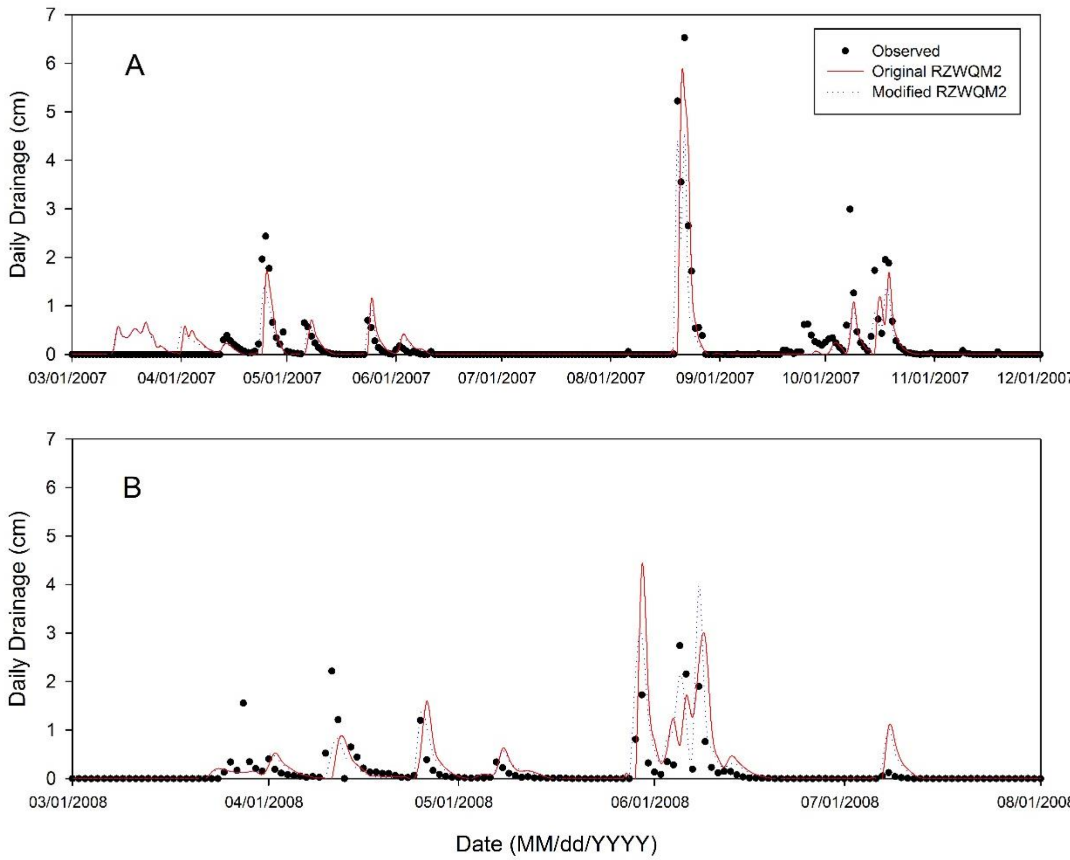

Figure 3. Iowa scenario: Observed daily drainage and daily drainage simulated by original and modified versions of RZWQM2 ($RZWQM2_0$ and $RZWQM2_R$) using the default Hooghoudt Equation (ssH): (A) 2007, (B) 2008.

Similar results were obtained from the simulations drawing on data from Ontario. Figure 4 shows observed and simulated drainage for all drainage periods during this two-year period. The *PBIAS* values were improved by modification of the model, decreasing from approximately 8% to 3% (Table 4). Besides of the lower bias, *NSE* and *IoA* were also improved in the modified model, *NSE* increased from 0.22, 0.22, and 0.19 to 0.36 0.31, and 0.32, and *IoA* increased from 0.65, 0.65, and 0.65 to 0.68, 0.67, and 0.67, for the three equations respectively (Table 4). The same pattern as was noted in Iowa could be found in Ontario scenario, the modified version $RZWQM2_R$

predicted cumulative drainage closer to observed values, and provided better peak drainage timing and distribution than $RZWQM2_0$. However, within a given version of RZWQM2 (both original and modified version), simulations with the three equations provided similar accuracy.

Table 3. Observed 2007-2008 Iowa cumulative drainage flow and equivalent values simulated with the original or modified $RZWQM2$ model using the steady-state equation (ssH) or the transient equations (inH and vanS), with model accuracy statistics (PBIAS, NSE and IoA) for daily drainage over the same period

Parameter	Observed	Simulated					
		Original ($RZWQM2_0$)			Modified ($RZWQM2_R$)		
		ssH	*inH*	*vanS*	*ssH*	*inH*	*vanS*
Cumulative drainage [mm (2 y)$^{-1}$]	810.4	920.9	931.6	931.6	862.8	862.3	862.4
Model accuracy statistics for daily drainage 2007-2008							
PBIAS	—	13.65%	14.96%	14.96%	6.48%	6.41%	6.42%
NSE	—	0.40	0.41	0.41	0.71	0.70	0.70
IoA	—	0.69	0.70	0.70	0.76	0.76	0.76

The modification improved model performance by simulating a better drainage distribution and peak timing in small time steps (Figure 2), which is critical to the simulation of the fate of agricultural contaminants in subsurface drainage. As the pesticides and herbicides penetrate into soil profile and are transported along with infiltrated water, the concentration of the contaminants in leachate is highly related to subsurface drainage peaks. A better simulation in peak timing will result in a more accurate prediction in the transport of contaminants, in particular for those with a short degradation half-life time, because the several hours delay of the simulated drainage peak could result in a high bias in the prediction in contaminants.

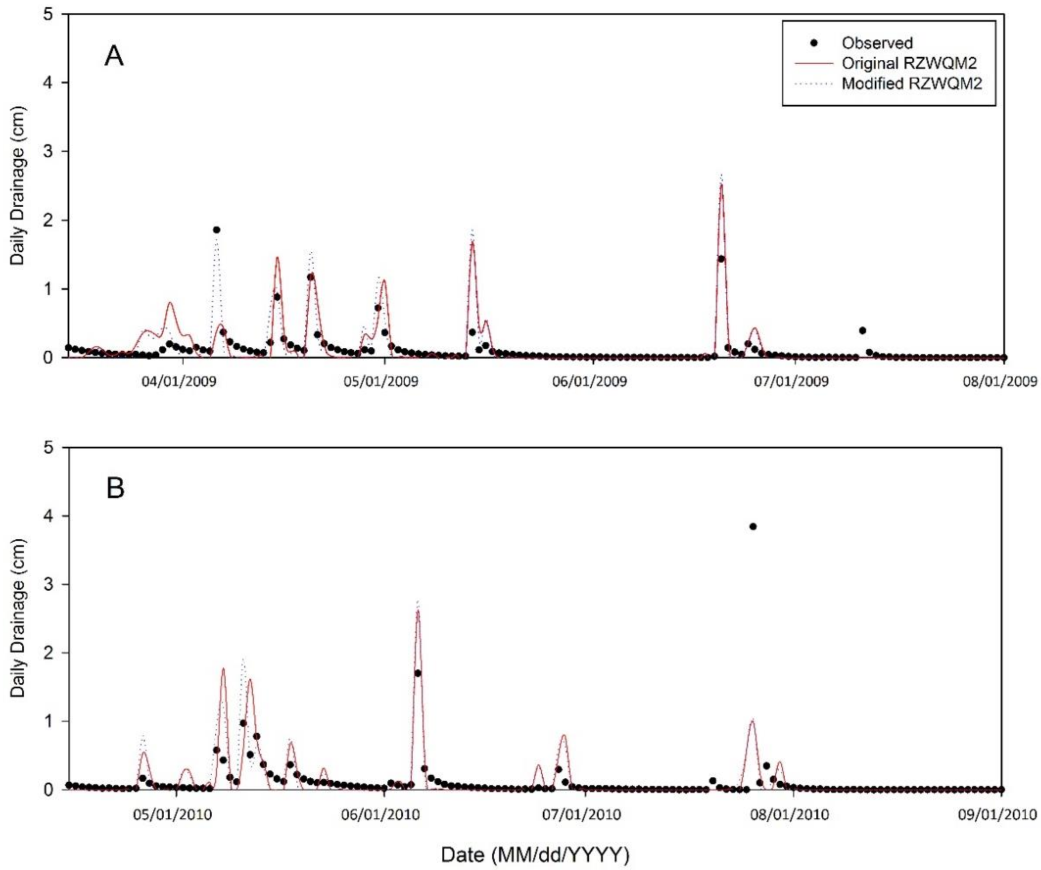

Figure 4. Ontario scenario: Observed daily drainage and daily drainage simulated by original and modified versions of RZWQM2 ($RZWQM2_0$ and $RZWQM2_R$) using the default Hooghoudt Equation (ssH): (A) 2009, (B) 2010.

Table 4. Observed 2009-2010 (non-freezing periods) Ontario cumulative drainage flow and equivalent values simulated with the original or modified $RZWQM2$ model using the steady-state equation (ssH) or the transient equations (inH and vanS), with model accuracy statistics (PBIAS, NSE and IoA) for daily drainage over the same period

Parameter	Observed	Simulated					
		Original ($RZWQM2_0$)			Modified ($RZWQM2_R$)		
		ssH	*inH*	*vanS*	*ssH*	*inH*	*vanS*
Cumulative drainage [mm (2 y)$^{-1}$]	318.7	347.0	346.9	340.1	329.0	330.1	328.2
Model accuracy statistics for daily drainage 2007-2008							
PBIAS	—	8.87%	8.86%	6.74%	3.34%	3.59%	2.98%
NSE	—	0.22	0.22	0.19	0.36	0.31	0.32
IoA	—	0.65	0.65	0.65	0.68	0.67	0.67

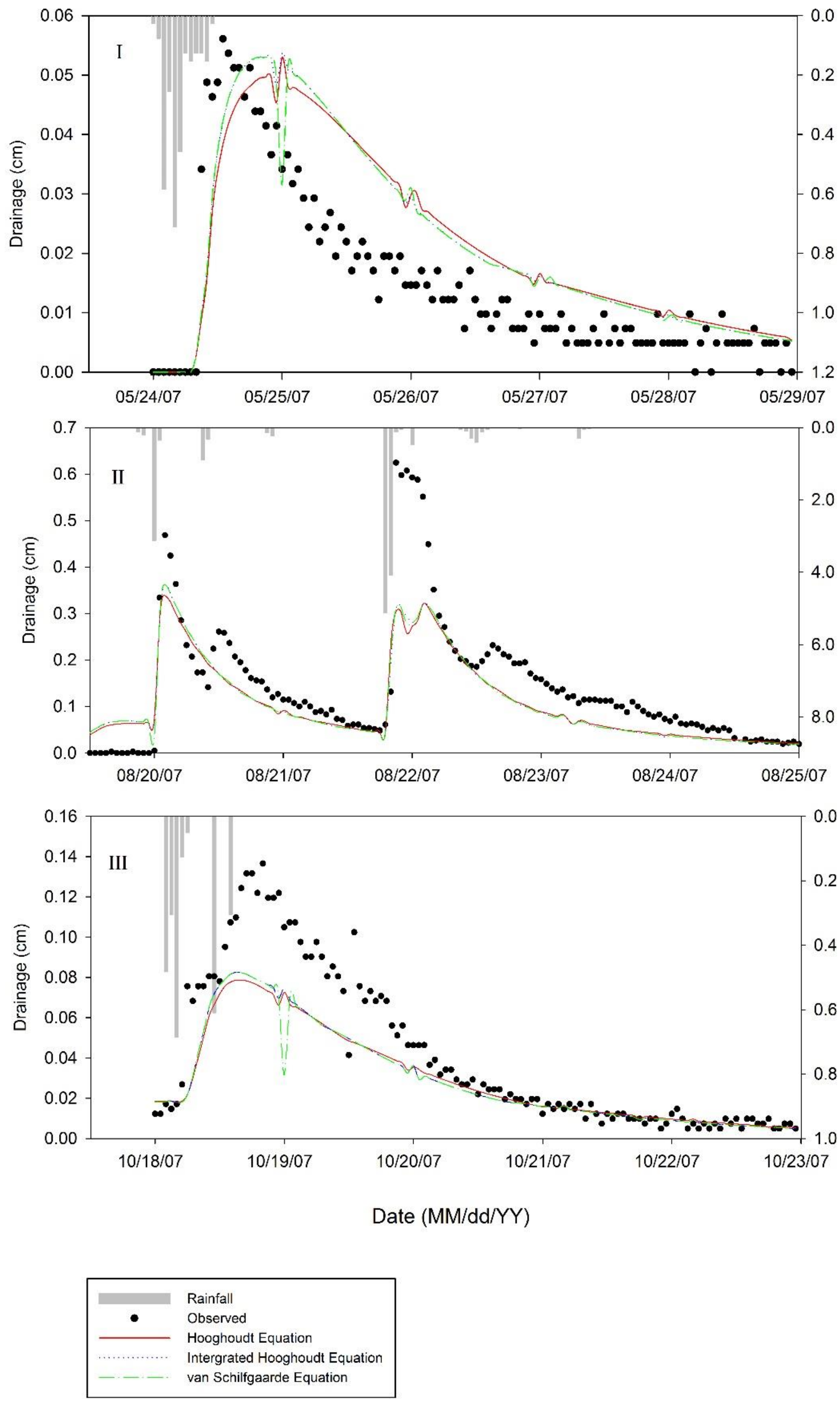

Figure 5. Hourly drainage comparisons in Iowa: observed and simulated by $RZWQM_R$ using the steady-state Hooghoudt equation (ssH), the transient integrated Hooghoudt (inH) or van Schilfgaarde (vanS) equations. I: Period (i) 24-28 May 2007, II: Period (ii) 19-25 August 2007 and III: Period (iii) 18-22 October 2007.

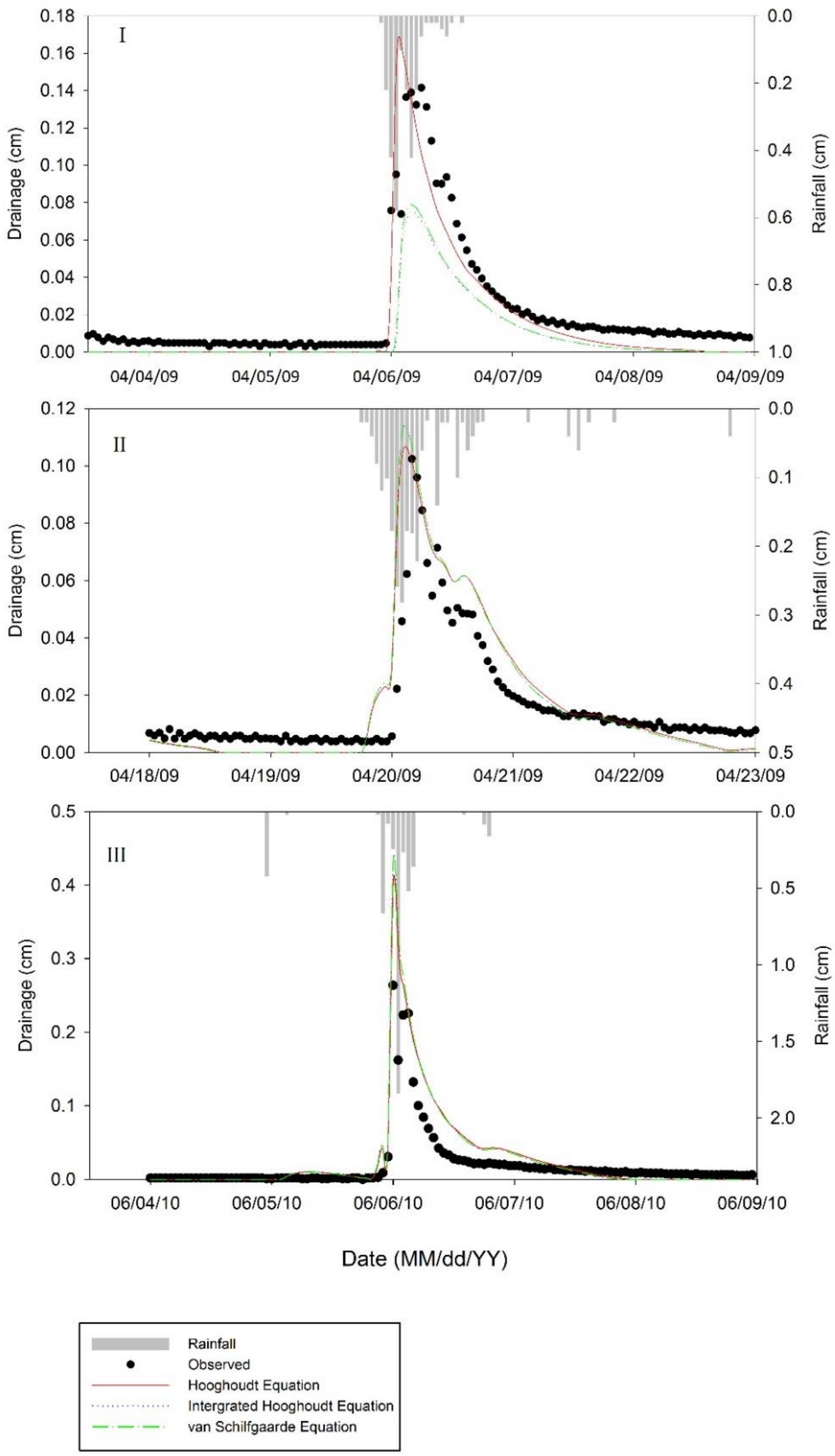

Figure 6. Hourly drainage comparisons in Ontario: observed and simulated by $RZWQM_R$ using the steady-state Hooghoudt equation (ssH), the transient integrated Hooghoudt (inH) or van Schilfgaarde (vanS) equations. I: Period (i) 4-8 April 2009, II: Period (ii) 18-22 April 2009 and III: Period (iii) 4-8 June 2010.

2.4.2 Transient Equations *vs.* Steady state equation

To explore the performance of these equations at a shorter time scale, hourly simulation results were plotted alongside hourly observed drainage data, and three typical and reasonable drainage periods were simulated under each scenario. In Iowa, the collected hourly periods were: (i) 24-28 May 2007, (ii) 19-25 August 2007, (iii) 18-22 October 2007 (Figure 5), while in Ontario they were: (i) 4-8 April 2009, (ii) 18-22 April 2009, and (iii) 4-8 June 2010 (Figure 6). Since the comparison between $RZWQM2_R$ and $RZWQM2_O$ showed that the modified version could provide better simulations, the hourly scale study in was therefore based on the modified version, in order to assess equations effects on well-simulated peaks.

Comparisons of $RZWQM2_R$ accuracy statistics across the three equations showed no significant differences; neither *PBIAS*, *NSE* nor *IoA* were obviously affected by the changes in drainage equation (Table 5). In Iowa, three predictions of drainage peaks from the *ssH*, *inH* and *vanS* equations are almost overlapping (Figure 5). Under the Ontario scenario (Table 5), the first period (Figure 6-I) showed a distinct difference in equation accuracies. The peak was well simulated by original *ssH* equation (*PBIAS* = -25.76%, *NSE* = 0.83, *IoA* = 0.81), while the *inH* (*PBIAS* = 58.03%, *NSE* = 0.59, *IoA* = 0.71) and *vanS* (*PBIAS* = 53.36%, *NSE* = 0.62, *IoA* = 0.72) equations significantly underestimated peaks and provided worse overall results. However, periods ii and iii followed the pattern of the Iowa scenario, where the three equations showed only negligible differences (Figure 6-II, III).

By comparing the observed and simulated values at a precise hourly time step, model performance was not satisfactory. Some peaks were not perfectly matched, for example, the second peak in Iowa period ii (Figure 5-II) was underestimated, which could be due to the saturated topsoil after the first rainfall event, or the infiltration process in the model underestimated the penetrating water in the second event, resulting at a lower simulated peak. Activating the macropore component in the model and allowing excessive surface water to penetrate into soil profile could solve the underestimation problem in this case.

Defects in simulation of peak drainage quantity and timing resulted in high PBIAS values at an hourly scale. These could be attributed the poor accuracy of model simulation and data measurement on a precise hourly scale. In addition, there were numeric instabilities in some hourly simulations (*e.g.*, *vanS* in Iowa period i and period iii, Figure 5-I, III). Since RZWQM2 uses Richards' equation to update soil water redistribution and determine the water table level, it might suffer from an instability in convergence of the iterative calculation occurring in some time steps.

Table 5. Statistics of evaluations for three equations (ssH, inH, vanS) on hourly scale in six drainage peak periods from Iowa and Ontario

			ssH	*inH*	*vanS*
Iowa	Period i	PBIAS	44.03%	45.16%	43.96%
		NSE	0.41	0.43	0.44
		IoA	0.61	0.62	0.62
	Period ii	PBIAS	-27.99%	-27.76%	-27.95%
		NSE	0.58	0.60	0.59
		IoA	0.76	0.76	0.76
	Period iii	PBIAS	-28.20%	-28.38%	-29.25%
		NSE	0.70	0.72	0.70
		IoA	0.80	0.81	0.80
Ontario	Period i	PBIAS	-25.76%	-58.03%	-56.36%
		NSE	0.83	0.59	0.62
		IoA	0.81	0.71	0.72
	Period ii	PBIAS	12.15%	12.03%	12.02%
		NSE	0.68	0.63	0.63
		IoA	0.74	0.73	0.73
	Period iii	PBIAS	47.11%	48.29%	48.37%
		NSE	0.61	0.53	0.53
		IoA	0.67	0.66	0.66

As for the evaluation of the three equations, our focus was more on their relative accuracy than their absolute accuracy. In general, the effects of different equations on peak simulations were very limited. In Ontario, for period i the original *ssH* showed a better performance than the other equations, likely because this was an early spring period (April 4^{th} 2009), temporally very close to the sub-zero period excluded from the test data. The discrepancy in soil water distribution compared to equation-derived levels could be linked to water accumulation in the sub-zero period, leading to greater inter-equation differences for the first peak period. However, in most of the cases in both Iowa and Ontario, the differences amongst equations were not significant, particularly between the two transient equations, and predicted and simulated hourly drainage nearly always overlapped closely. An analysis of hourly results indicates that the two transient state drainage equations provided no significant improvement to the model, so that the original *ssH* equation was suitable in hourly drainage simulation, providing acceptable results.

Singh et al. (1992) drew similar conclusions after testing various transient equations to predict falling water tables: all equations employed generated similar reasonable estimates of falling water table heights when compared to observed values. Other studies have evaluated steady- and unsteady-state equations in simulating drainage spacing and drainage flow (Darzi-Naftchally et al., 2012; Kumar et al., 2012) and generally concluded that unsteady state equations were more suitable under their field conditions. The most likely reason for this is the model's time step: in RZWQM2 the time step ranges from 10-5 to 0.1 hour depending on the convergence of Richards' equation in daily physical processes. After each tiny time step, the water table height is updated according to the drainage rate and soil water movement; therefore, even steady state equations assume the water table height not to fluctuate over such a duration, i.e., this assumption's effects are minor since the time step is short enough. Thus, the differences between these two kinds of drainage equations in RZWQM2 is not significant. In addition, differing field soil conditions in different studies may also affect drainage equations' simulations.

2.5 Conclusions

This study modified the soil water redistribution and tile drainage processes in RZWQM2. Based on statistical results, the modified version significantly enhanced model performance compared with the original RZWQM2. Two types of drainage equations: steady state (*ssH*) and unsteady-state (*inH* and *vanS*) were tested with both the original ($RZWQM2_0$) and the modified form of the model ($RZWQM2_R$), where rainfall and soil water redistribution were allowed to occur simultaneously when modeling drainage under long duration rainfall events. The improvement in drainage peak timing simulation benefits RZWQM2 to have better performance in modeling agricultural contaminants in short time scale. Although based on different assumptions, the transient and steady state equations implemented in RZWQM2 provide very similar predictions in most cases. No differences in model drainage simulation performance were noted among the three equations or between the two unsteady-state equations. Approaches in this study ($RZWQM2_0^{ssH}, RZWQM2_0^{inH}, RZWQM2_0^{vanS}, RZWQM2_R^{ssH}, RZWQM2_R^{inH}, RZWQM2_R^{vanS}$) tend to underestimate the peak values and do not simulate the drainage distribution very well in some of the hourly cases. For further investigation, introducing macropore preferential flow could be an effective way, which not only provides extra channels for excessive water to penetrate, but also allow faster drainage peak occurrence and lateral infiltration. More future work can be focus on macropore flow simulation in RZWQM2 to improve drainage peak predicting in high time resolution. In addition, data from different climates, soil properties and agronomic management practices should be tested to further evaluate these equations, and alternate approaches should be tested to improve model performance in simulating drainage peaks.

Connecting Statement to Chapter 3

In Chapter 2, we solved peak delay problem in RZWQM2 and significantly improved model performance in short time simulations. However, neither the modified model nor the transient equations improved the simulated peak values. There are obvious underestimations in simulated peaks.

In Chapter 3, macropore component in RZWQM2 was activated and calibrated in two scenarios, based on hourly observed data from Iowa and Ontario. This study aims at testing the effectiveness of macropore component in improving drainage peak simulations in short time scale.

Chapter 3 is a manuscript prepared for publishing in related domain's journal in future. The manuscript is co-authored by my supervisor Dr. Zhiming Qi, and also Dr. Chin S. Tan, Dr. Tiequan Zhang.

Chapter 3. Testing Macropore Component of RZWQM2 in Subsurface Drainage Peak Simulation on Hourly Time Scale

3.1 Abstract:

A solid understanding of preferential flow through soil macropores, a key element of the hydrological cycle, is critical to an effective management of the quality of subsurface drainage water flowing from agricultural fields. However, the measurement of the size and distribution of macropore is difficult, costly, and laborious. The ability of the Root Zone Water Quality Model (RZWQM version 2.94.00) to predict drainage peaks on a short time scale was assessed both with and without its macropore component. The model was independently calibrated with field data from each of two experimental sites: Ontario, Canada (2008-2011), and Iowa, USA (2007-2008). For three drainage peaks recorded at the Ontario site, the inclusion of the model's macropore component improved the simulation of drainage peak magnitude, reducing the percent bias (PBIAS) from 51.59% ≤ PBIAS ≤ 39.97% to 31.35% ≤ PBIAS ≤ 11.28%. In contrast, for a single period/peak at the Iowa site, inclusion of the model's macropore component worsened the simulation, increasing the magnitude of the PBIAS from -51.92% to 67.63%. Overall, the general performance of the macropore component equipped model proved unsatisfactory due to an overly delayed simulated drainage recession. For the peaks in Ontario, upon inclusion of the macropore component, the Nash-Sutcliffe Efficiency (NSE) dropped from 0.47 ≤ NSE ≤ 0.54 to 0.25 ≤ NSE ≤ 0.46 in all peak periods decreased from, while the Index of Agreement (IoA) decreased from 0.58 and 0.77 to 0.52 and 0.75 for the two peaks (Period 1) in Ontario, and increased from 0.68 to 0.71 for the single peak studied in Iowa. Two important parameters: Predicted total macropore flow and drainage peaks proved to be insensitive to macroporosity and pore radius, a 50% change

in the latter, resulting in a <5% change in the former. Addition of a macropore component to the model allowed it to better mimic drainage peaks during excess surface flow events, but did not provide sufficient accuracy in representing the real macropore flow process, to forestall further investigation and model modifications targeted towards improving RZWQM2's hydrologic simulation of macropores.

Keywords:

Macropores, Preferential flow simulation, Subsurface drainage modeling, RZWQM2.

3.2 Introduction

Found predominantly in field soils, macropores are visible open channels with relatively large diameters (ranging from very fine, 70 μm < D <1000 μm, to coarse, D > 5.0 mm), and capable of extending continuously, vertically or horizontally, over a significant length (L > 150 mm), thereby connecting lower soil horizons and the soil surface (Beven *and* Germann, 1982). However, given their different origins, as well as their morphologic and structural properties, their size can vary widely (Omoti *and* Wild, 1979; Mosley, 1982; Peron *et al.*, 2009). Macropores can be formed under various circumstances, including burrowing animals, plant roots, soil drying cracks, etc. (Beven *and* Germann 2013). In addition, the structure and composition of macropores remain in a constantly evolving dynamic balance, which varies with changes in climate, biological community and anthropogenic land use. A number of studies investigating the formation, age and changes of macropores (Beven *and* Germann, 1982; Green *and* Askew, 1965) suggest that, depending on soil texture and composition of the soil's organic matter, their effective lifetime under stable conditions can extend into hundreds of years (Beven *and* Germann, 1983). In general, macroporosity is higher in undisturbed soil, and conversely, lower and shorter-lived at sites under agricultural production, where they may only last until the next tillage.

Quantified using different measurement techniques and flow processes, pore size and structure are two widely ranging but nonetheless important criteria in describing macropores. Though macropores do not necessarily occupy large voids in the soil, they can significantly affect soil hydraulics and soil water movement, thereby allow soils to exhibit non-equilibrium channel flow (Brewer, 1980; Reeve *et al*., 1980). In the presence of soil macropores, the capillary tube analogy in soil hydraulics and the steady equilibrium assumptions of Darcy and Richards equations may not be suitable to simulate water movement through soils (Beven *and* Germann 2013). Subsurface drainage waters draw on two sources: (i) water having directly travelled through opening channels (*i.e*., macropores), and (ii) water discharged from a saturated soil matrix. Water can be drained out through macropores when the surrounding soil profile is already saturated, or macropore flow can be so rapid as to allow water to pass through the soil before being absorbed (Lawes *et al*., 1882). Compared with equilibrium flow in a soil matrix, which is driven by equilibrium potentials, water flow in macropores is much faster. Since macropores provide water an express channel, a larger fraction of macropores in a soil may account for a faster drainage velocity and ultimately, a greater quantity of water drained.

Besides their influence on drainage water volume, macropores also affect drainage water quality (Allaire-Leung *et al*., 2000). Water carrying solutes, chemicals or contaminants will interact less with surrounding soil when passing through macropores, resulting in a higher proportion of solutes being discharged without interacting significantly with the soil matrix, thereby raising the concentration of contaminants and offering faster leaching through drainage water. Many studies were conducted to investigate solute transportation in macropores flow

(Kladivko *et al*., 1991; Stamm *et al*., 1998; Simard *et al*., 2000), have shown that macropores and preferential flow have a significant impact on herbicide and pesticide transportation, and should therefore be considered as an important factor in drainage water quality.

However, it is difficult to accurately determine the macropore density and structure in fields. While impregnation and sectioning techniques have been used to determine pore size (Hewitt *and* Dexter, 1980), they do little to provide information regarding macropore channels and structures. Fleming and Bradshaw (1992) developed a method to demonstrate presence of soil macropores in farmland using the surface emergence of smoke from smoke bombs and blowers placed beneath the soil surface. This technique is helpful for farmers to notice macropores in their field and may estimate possible macropore flow, but it is limited to describing macropore structure qualitatively. By using X-ray computed tomography, graphic analysis and 3-D reconstruction techniques to quantify macropores, a number of studies achieved more satisfactory results (Perret *et al*., 1999; Hu *et al*., 2014; Meng *et al*., 2015). While this has become a mature and acceptable method to measure macropores, these techniques are very demanding in terms of their hardware and software requirements, making them difficult to apply in general field studies.

Other methods to determine macropores properties include tension infiltrometers (Everts *and* Kanward, 1993), the suction plate method, dye tracers (Bouma *and* Wosten, 1979) and lab soil column experiments (Akay *et al*., 2008). However, no unified approach has proved satisfactory and easy to apply, so more macropores characterization techniques should be evaluated (Liu *et al*., 2014).

Mathematical models are potential solutions to identify macropores quantitatively. Many verified hydrological models have incorporated a macropore component to simulate preferential flow and attendant contaminant transportation. These models include HYDRUS, RZWQM2, MACRO, and PEARL. The macropore component in RZWQM2 has been proven to be satisfactory in simulating herbicide and pesticide transportation. Kumar *et al.* (1998) showed that by activating the macropore routines in RZWQM2, hydraulic properties of soil profile were changed, and a more accurate prediction of herbicide concentration in drainage was achieved, along with a slightly improved prediction of daily subsurface drainage flow.

However, the model's macropore component has not been widely used in hydrological simulations yet, since its effect on overall drainage is negligible, and the performance of the macropore component in short periods with a high time resolution (*e.g.*, hourly) has not been investigated. Since it is only activated when excess surface flow exists, it is no surprise that the macropore component makes little difference to simulations on daily or annual time scales. The change in macropore flow is insignificant compared with the long term drainage quantity. However, given the presence of plant roots, burrowing animals and tillage operations in agricultural lands, macropores should not be excluded from simulations.

There is some evidence implying that the inclusion of a macropore component would improve model performance for short-term drainage events. The macropore-component-free RZWQM2 model has shown a tendency to underestimate peak values of subsurface drainage (Kumar *et al*., 1998; Qi *et al*., 2011), which could be due to it ignoring soil macropores. High drainage peaks usually follow a rainfall event, however, when the recharge rainfall is excessive or rapid, the simulated infiltration rate would be limited by Green-Ampt equation, resulting in less infiltrated water and lower drainage. Alternatively, inclusion of a macropore component in the model can provide channels for excess surface water to enter the soil profile, which more closely mimics the real situation and may, accordingly, allow a better simulation of drainage peak values.

Therefore, one of the present study's goals was to test the macropore component of RZWQM2 at an hourly time step, focusing on drainage peak periods where the macropore component would be activated. The specific objectives of this study were: (i) to calibrate RZWQM2 with the macropore component using observed data from Iowa and Ontario, and then evaluate the model performance in simulating drainage peaks, (ii) to test the sensitivity of the macropore-component-activated model's outputs to two important macropore model component parameters: macroporosity and pore radius.

3.3 Materials and Methods

3.3.1 Ontario and Iowa Drainage Sites

Table 6. Peak drainage flow periods and individual events employed in hourly analysis of RZWQM2 model accuracy (with and without its macropore component) for peak flow scenarios at Iowa and Ontario sites

Site	Peak designation	Period		Peak		
		No.	Date of Period	No.	Time	Observed Peak Drain Flow Rate (mm hr^{-1})
Iowa	$P_{1\text{-}1}^{Iowa}$	1	19th – 23rd August, 2007	1	21st August, 2007 20:00	6.0
Ontario	$P_{1\text{-}1}^{Ont}$	1	27th – 29th June, 2008	1	28th June, 2008 1:00	4.6
	$P_{1\text{-}2}^{Ont}$	1	27th – 29th June, 2008	2	28th June, 2008 15:00	5.2
	$P_{2\text{-}1}^{Ont}$	2	25th – 27th May 2011	1	26th May, 2011 10:00	4.0

Two sets of data were used to assess the contribution of the macropore component of the RZWQM2 model. The first experiment was conducted by Tan *et al*. (2009), at an experiment field located on the north shore of Lake Erie near Harrow, Ontario. The second field study was conducted at the Agricultural Drainage Water Quality – Research and Demonstration Site (ADWQ-RDS) near Gilmore City in Pocahontas County, north central Iowa. To assess the effects of considering macropores on the accuracy of high resolution time scale drainage peak simulation, we selected three periods (two from Ontario and one from Iowa) during which macropore flow occurred, and within which four drain flow peaks equal to or exceeding 4.0 mm hr^{-1} occurred (Table 6).

Initiated in spring 2008, the experimental site in Ontario consisted of 16 (131 m × 25 m) drained plots (Tan *et al*., 2009). Buffer zones and impermeable barriers were set to prevent interaction amongst plots. In this study, two plots with regular drainage were used to test the macropore component of RZWQM2. The predominant soil in these fields was a Brookston clay loam, with a mean of 28% sand, 37% silt and 35% clay, a mean bulk density $\rho = 1.34$ Mg m^{-3}. The measured soil porosity was 52.4% and k_{sat}^{ver} ranged from 17 to 119 mm d^{-1}, with an average 50 cm d^{-1} (Liu *et al*., 2011). Hourly observed drainage outflow volumes from the two experimental plot recorded during 2008 and 2012, were average across plots. Hourly weather data including precipitation, air temperature, solar radiation, wind speed and relative humidity were recorded at the Whelan weather station, located less than 0.5 km from the experiment site. However, the rainfall measurements for the period of Oct 1st 2008 to April 30th 2009 being unavailable at the Whelan station were drawn from the Harrow weather station located 16.6 km from the site.

Initiated in fall 2004 and continued for five years, the Iowa field experiment was arranged in a completely randomized block design with 78 individually-drained plots (Lawlor *et al*., 2008) replicated in each of four blocks selected for their contrasting long-term drainage performance (*e.g*., high, medium-high, medium-low and low drainage). In each block, plots were randomly assigned a specific land use/land cover treatment, resulting in each treatment — in this case corn (odd year)-soybean (even year) rotation, winter wheat crop incorporated at planting each year — being repeated four times. Hourly drainage from each plot was monitored, and the mean values across the four plots served as the observed hourly drainage data used in this study.

The hydraulic properties, bulk density (ρ), particle size distribution, saturated hydraulic conductivity (k_{sat}) and soil water characteristic curves of the predominantly fine loam (USDA 1985) soils were determined from undisturbed soil cores (Table 7). Bubbling pressure and pore size distribution were fit using the Brooks-Corey equation (Brooks *and* Corey, 1964). Residual water content, and soil moisture (θ) at different matrix potentials (10, 33 and 1500 kPa) were interpolated or extrapolated from the soil water characteristic curve. During the five-year experiment period, hourly meteorological data including rainfall, air temperature, solar radiation, relative humidity and wind speed were monitored by an onsite weather station.

3.3.2 Macropore component in RZWQM2

Developed in 1993, the macropore component in RZWQM2 was included to allow the simulation of preferential flow in agricultural lands. The soil parameters necessary to the operation of this component include sorptivity factor, marcopore to tile drain expression fraction and effective lateral infiltration wetting thickness. In addition, for each soil horizon, macropore-related parameters include macroporosity, pore radius, width and length of crack, length of aggregate and fraction of dead end pores. Macropores are considered as cylindrical pores in top layers and as cracks in lower layers (USDA-ARS, 1992; Ahuja *et al.*, 2000). The macroporosity and pore radius in each layer are core parameters required by this model component, which describe the macropores quantitatively and determines the total number of pores in the field. Depending on these two parameters, RZWQM2 computes the density of macropores per unit area as (USDA-ARS. 1992):

$$n_{macro} = \frac{MP}{\pi r^2} \tag{19}$$

where,

n_{macro}	is the number of macropores in per unit area, which are assumed to be evenly distributed in the soil layers,
r	is the radius in each soil horizon within which macropores are found (mm), and
MP	is the macroporosity in each soil horizon ($mm^3\ mm^{-3}$).

When the model is recharging water from rainfall or irrigation, the water is first considered to infiltrate into the soil matrix first using Green-Ampt equation, as macropores contribute very small fraction of the total surface area. The excess surface flow, which would be considered as runoff when ignoring macropores effects, is allowed to enter macropores along with the solutes it bears. Based on Poiseulle's law, the maximum capacity of macropore flow ($cm\ h^{-1}$) for the upper (K_{mac}^{up}) and lower (K_{mac}^{low}) soil layers were computed as:

$$K_{mac}^{up} = \frac{P_{mac}^{up}\,\rho g r^2}{8\eta} \tag{20}$$

$$K_{mac}^{low} = \frac{P_{mac}^{low}\,\rho g d^2}{12\eta} \tag{21}$$

where,

d	is the width of planar cracks (mm) in the lower soil layer,
g	is the gravitational constant ($mm\ h^{-2}$),
r	is the radius of cylindrical pores (mm) in the upper soil layer,
$P_{mac}^{up}, P_{mac}^{low}$	are the macroporosities ($mm^3\ mm^{-3}$) of the upper and lower soil layers, respectively,
η	is the dynamic viscosity of water ($g\ mm^{-1}\ h^{-1}$), and
ρ	is the density of water ($g\ mm^{-3}$)

Continuous macropores are assumed to extend vertically in soil, and a portion of them to be blocked at each soil horizon according to the dead end pores parameter set by the user. According to the value of the sorptivity factor, water flowing through macropores can be absorbed to a greater or lesser degree by the surrounding unsaturated soil matrix. Derived through the lateral

Green-Ampt equation (Kumar *et al*., 1998), the infiltration rates (cm h^{-1}) for the upper (V_{up}) and lower (V_{low}) soil layers were computed as:

$$V_{up} = 2\pi r\sqrt{\frac{2k_{sat}H_c(\theta_{sat} - \theta_i)}{0.5\Delta t_1}} \tag{22}$$

$$V_{low} = \sqrt{\frac{2k_{sat}H_c(\theta_{sat} - \theta_i)}{t}} \tag{23}$$

where,

k_{sat}	is the saturated hydraulic conductivity (cm h^{-1})
Δt_1	is the first time step in model calculation (h)
t	is the cumulative time for lateral flow (h)
H_c	is the capillary drive term for the soil matrix (cm)
$(\theta_{sat} - \theta_i)$	soil moisture deficit in the particular soil depth range, namely the soil moisture content at saturation (θ_{sat}) minus the soil moisture under present conditions (θ_i) (cm^3 cm^{-3})

The water reaching a dead end can be absorbed or stored, while the remaining water will be routed to the water table. When the macropore flow first reaches the top of the water table, a small fraction of water, bearing the initial solute concentration, is assumed to go directly to the tile drains, such that the solutes are not diluted by ground water, thereby avoiding the underestimation of solute concentrations in drainage water (Fox *et al*., 2004; Malone *et al*., 2001).

3.3.3 Parameterization for the Ontario scenario

Lu (2015) calibrated RZWQM2 based on measured subsurface drainage and surface runoff data at the Ontario site in which the experimental period (from June 1st to Dec 22nd 2011) was divided into 17 time spans (Table 7). Input parameters were calibrated to match the periodic observations in those 17 time spans. In this study, we recalibrated the hydraulic parameters to match hourly observations (Table 8), based on a previous study by Lu (2015).

Table 7. Sampling time spans for drainage measurements in Ontario

Sampling Spans	Duration	
	From	To
1	June 1, 2008	June 16, 2008
2	June 17, 2008	July 17, 2008
3	July 18, 2008	October 22, 2008
4	October 23, 2008	February 11, 2009
5	February 12, 2009	March 27, 2009
6	March 28, 2009	May 26, 2009
7	May 27, 2009	July 17, 2009
8	July 18, 2009	October 23, 2009
9	October 24, 2009	April 20, 2010
10	April 21, 2010	June 11, 2010
11	June 12, 2010	August 5, 2010
12	August 6, 2010	December 21, 2010
13	December 22, 2010	March 23, 2011
14	March 24, 2011	June 22, 2011
15	June 23, 2011	September 7, 2011
16	September 8, 2011	November 9, 2011
17	November 10, 2011	December 22, 2011

Table 8. Calibrated soil hydraulic properties at the Ontario site

Depth (m)	ρ (Mg m^{-3})	*Sand* (g g^{-1})	*Silt* (g g^{-1})	K_{sat}^{ver} (mm h^{-1})	K_{sat}^{lat} (mm h^{-1})	Soil moisture content, θ (mm^3 mm^{-3}) Soil matric potential, ψ_m (kPa)				
						θ_{sat} 0 kPa	θ_{10} -10kPa	θ_{fc} -33 kPa	θ_{pwp} -1500kPa	θ_r -∞ kPa
0-0.25	1.326	0.299	0.363	9.2	17	0.5	0.383199	0.325024	0.198328	0.04
0.24-0.45	1.391	0.238	0.349	38	68	0.475	0.378326	0.336288	0.23956	0.09
0.45-0.80	1.391	0.257	0.33	30	60	0.475	0.370845	0.329898	0.23568	0.09
0.80-1.20	1.391	0.243	0.359	20	40	0.475	0.390282	0.346501	0.245762	0.09
1.20-3.00	1.391	0.243	0.359	5	20	0.475	0.390282	0.346501	0.245762	0.09
3.00-3.09	1.391	0.243	0.359	0.1	20	0.475	0.390282	0.346501	0.245762	0.09

Note: ρ = soil bulk density; Sand (50–2000 μm) and Silt (2–50 μm) fractions; $k_{\mathrm{sat}}^{\mathrm{ver}}$ and $k_{\mathrm{sat}}^{\mathrm{lat}}$, vertical and lateral saturated hydraulic conductivity, respectively. θ_{sat}, θ_{fc}, θ_{pwp}, are soil moisture at saturation, field capacity and permanent wilting point, respectively. θ_r is the residual soil water content.

For the Ontario site, macroporosity and pore radius were quantified based on hourly drainage observations. The lengths of cracks and aggregates were assumed to decrease with soil depth, while dead end pore fractions increased. The parameters of sorptivity factor and expression fraction were set to the same values as for the Iowa field (0.5 and 0.02, respectively). All other parameters were calibrated to match hourly observed drainage flow peaks over the full experiment period (Table 9).

Table 9. Parameters of the RZWQM2 macropore component at the Ontario site

Soil depth (m)	macroporosity ($mm^3\ mm^{-3}$)	radius of cylindrical pores (mm)	width of rectangular cracks (mm)	length of cracks (mm)	average length of aggregate (mm)	fraction of dead end pores
0-0.25	0.0003	1	0	0	100	0.01
0.25-0.45	0.0003	0	1	100	100	0.3
0.45-0.80	0.0003	0	1	50	50	0.5
0.80-1.20	0.0003	0	1	50	50	0.8

3.3.4 Parameterization for the Iowa scenario

Soil hydraulics parameters for RZWQM2 were measured or calibrated by Qi *et al*. (2011) on a daily scale without consideration of macropore flow (Table 10). The ρ, particle size distribution and k_{sat} (i.e., vertical hydraulic conductivity k_{sat}^{ver}) were drawn from field measurements, and lateral saturated hydraulics conductivities (k_{sat}^{lat}) in each layer were adjusted to $2k_{sat}^{\text{ver}}$, in order to match the peaks of daily drain flow. Soil water retention curve parameters were measured in laboratory using soil columns but were calibrated to better match measured θ values.

In scenarios where the model's macropore component was activated, parameters for macropore component were calibrated using hourly drain flow data (Table 11). Macropores were assumed to exist in upper soil layers, where macropores can be formed by plant roots, burrowing animals and tillage activities, and it was assumed that no macropore occurred in soil layers deeper than 1.20 m. The parameters including sorptivity factor (set at 0.5), expression fraction (set at 0.02) and dead end pore fraction (Table 11) were also adjusted based on calibrated values from Kumar *et al*. (1998), and lengths of cracks and aggregates were based on default values in RZWQM2. In this study, lengths of cracks, aggregates, and proportion of dead end pore were not uniformly distributed in soil layers, with increasing soil depth, the average lengths of macropores were assumed to decrease and the dead end pore fraction to increase. The two key parameters — macroporosity and radius — were then calibrated to match hourly drain flow peaks.

Table 10. Calibrated soil hydraulic properties at the Iowa site

Depth (m)	ρ (Mg m^{-3})	*Sand* (g g^{-1})	*Silt* (g g^{-1})	k_{sat}^{ver} (mm h^{-1})	k_{sat}^{lat} (mm h^{-1})	Soil moisture content, θ (mm^3 mm^{-3}) Soil matric potential, ψ_m (kPa)				
						θ_{sat} 0 kPa	θ_{10} -10kPa	θ_{fc} -33 kPa	θ_{pwp} -1500kPa	θ_r -∞ kPa
0-0.10	1.37	0.32	0.36	48	97	0.482	0.383	0.376	0.1887	0.0705
0.10-0.20	1.38	0.32	0.36	33	66	0.476	0.384	0.376	0.2304	0.0718
0.20-0.30	1.39	0.33	0.53	51	101	0.473	0.384	0.376	0.2005	0.0787
0.30-0.40	1.39	0.40	0.30	40.8	82	0.474	0.384	0.399	0.2115	0.0721
0.40-0.60	1.39	0.46	0.30	40.8	82	0.474	0.408	0.368	0.2178	0.0645
0.60-0.90	1.45	0.44	0.34	26.4	53	0.450	0.380	0.368	0.2038	0.0339
0.90-1.20	1.46	0.44	0.34	26.4	53	0.450	0.312	0.299	0.1844	0.0325
1.20-2.00	1.46	0.44	0.34	26.4	53	0.450	0.310	0.299	0.1678	0.0325
2.00-3.00	1.5	0.44	0.34	26.4	53	0.450	0.310	0.299	0.1678	0.0325
3.00-3.90	1.5	0.44	0.34	0.001	50	0.450	0.310	0.299	0.1678	0.0325

Note: ρ = soil bulk density; Sand (50–2000 µm) and Silt (2–50 µm) fractions; $k_{\mathrm{sat}}^{\mathrm{ver}}$ and $k_{\mathrm{sat}}^{\mathrm{lat}}$, vertical and lateral saturated hydraulic conductivity, respectively. θ_{sat}, θ_{fc}, θ_{pwp}, are soil moisture at saturation, field capacity and permanent wilting point, respectively. θ_r is the residual soil water content.

Table 11. Calibrated parameters of the macropore component for the Iowa site

Soil depth (m)	Macroporosity (mm^3 mm^{-3})	Radius of cylindrical pores (mm)	Width of rectangular cracks (mm)	Length of cracks (mm)	Average length of aggregate (mm)	Fraction of dead end pores
0-0.10	0.001	2	0	0	100	0.001
0.10-0.20	0.001	0	2	100	100	0.01
0.20-0.30	0.001	0	2	100	100	0.05
0.30-0.40	0.001	0	2	100	50	0.1
0.40-0.60	0.001	0	2	50	50	0.3
0.60-0.90	0.001	0	2	50	50	0.5
0.90-1.20	0.001	0	2	50	50	0.8

3.3.5 Sensitivity test

Since macropores vary widely, the calibrated parameters may not apply to all field conditions; therefore, sensitivity tests were conducted to analyze the effects of changing the macropore parameters of macroporosity and pore radius on simulation results. Because macroporosity and pore radius vary independently, under different conditions, the sensitivity analysis therefore included a large range of parameter variation, from 50% to 150% of the original value (i.e. the calibrated values in each scenario), while other parameters were kept unchanged. The analysis was conducted in several periods of high flow rate instead of over whole years, because in the model the macropore component calculations are only implemented during a few excessive water events during the whole period, and the change in macropore flow is tiny compared to the total drainage volume.

In addition, to analyze macropore parameters effects on simulating hourly drainage peaks, sensitivity tests were conducted in specific peak periods. For each of the two parameters, within the range 50% to 150% of original value we sampled 10 values with equivalent increments, and then factorially combined the 10 values of the two parameters as model inputs, therefore generating 100 tests for each drainage peak period. The performance of the macropore component in matching drainage peaks and sensitivity of parameters were analyzed based on the means and standard errors from the 100 tests.

3.3.6 Statistical methods for model accuracy evaluation

To evaluate the performance of the model, the percent of bias (PBIAS), Nash-Sutcliffe efficiency (NSE) and Index of Agreement (IoA) were used:

$$PBIAS = 100 \cdot \frac{\sum_{i=1}^{n}(S_i - O_i)}{\sum_{i=1}^{n} O_i} \tag{24}$$

$$NSE = 1 - \frac{\sum_{i=1}^{n}(O_i - S_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \tag{25}$$

$$\mathrm{IoA} = 1 - \frac{\sum_{i=1}^{n}|S_i - O_i|}{2\sum_{i=1}^{n}|O_i - \bar{O}|} \tag{26}$$

where,

n	is the number of measured (or simulated) values,
O_i	is the i^{th} observed value,
$\bar{O}$	is the mean observed value,
S_i	the i^{th} simulated value.

In the drainage flow simulation, *PBIAS* within ±15%, *NSE*>0.70, and *IoA* close to 1 indicate the performance is good for a daily time step in RZWQM2 (Moriasi *et al.*, 2015), these criterions are used to evaluate model modifications in daily time scale. However, in hourly scale comparisons, the criterion for statistics are not available, we are comparing the differences of *PBIAS*, *NSE* and *IoA* between modeling methods to assess results.

3.4 Results and Discussions

3.4.1 Comparison between Simulations with and without macropores in Ontario

The effects of the presence/absence of RZWQM2's macropore component on simulated drain flow for all drainage spans (Table 7) between June 1st 2008 and December 22nd 2011 were evaluated (Figure 7; Table 12). In these long-term simulations with macropore component (MP) and without macropore component (NoMP) were not significantly different over the 17 periodic observations. While total drainage volume was underestimated with the NoMP model, the MP model which provided channels for more water to penetrate, only provided a small improvement in predicted total drain flow with 6% increase in total predicted drainage. The NSE and IoA, which describe the drainage flow distribution and pattern, were slightly decreased after activating the macropore component. NSE dropped from 0.48 to 0.46, and IoA dropped from 0.74 to 0.72. However, the changes in these two statistics were not significant (within 5% of the original values), because only a few events over the full simulation had water flow into macropores.

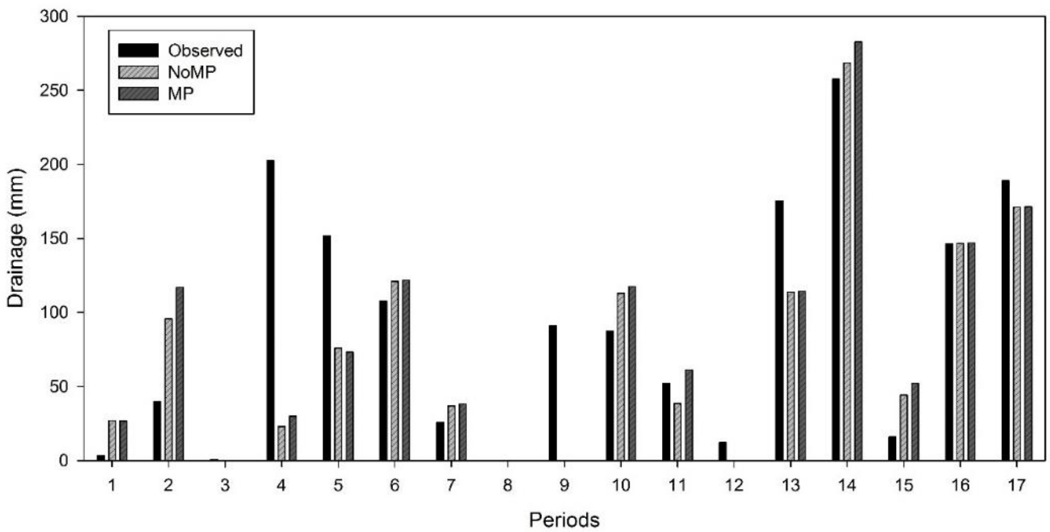

Figure 7. Observed cumulative drainage flow and predicted drainage flow by no macropore (NoMP) and with macropore (MP) RZWQM2 models for all sampling spans at the Ontario experimental site.

Table 12. Model accuracy statistics for no macropore (NoMP) and with macropore (MP) in long term drainage simulation, Ontario site

Model accuracy statistic	Cumulated Drainage (mm)		
		Simulated	
	Observed	NoMP	MP
	1558.6	1275.0	1353.0
PBIAS		-18.20%	-13.19%
NSE		0.48	0.46
IoA		0.74	0.72

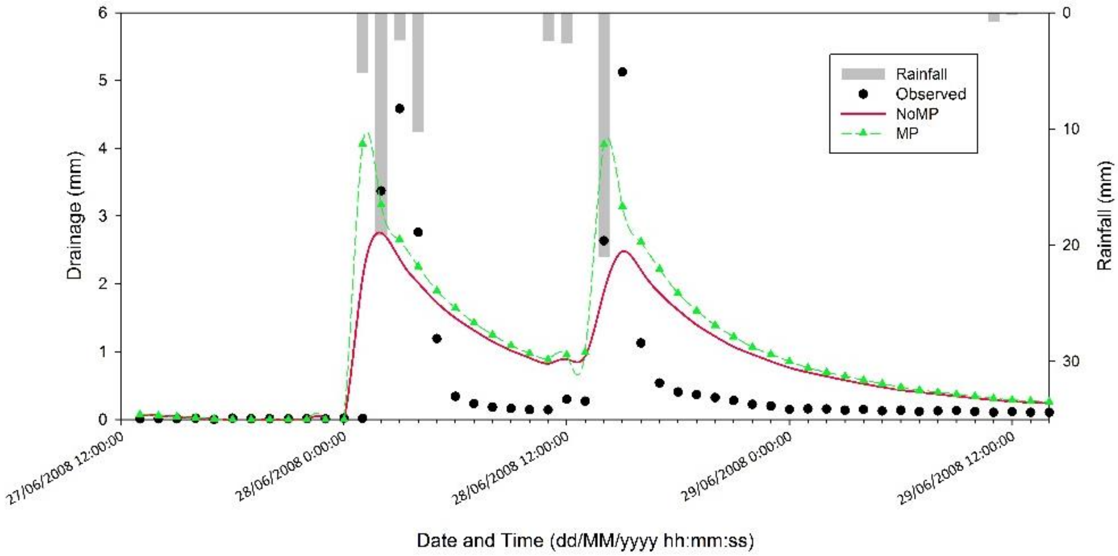

Figure 8. Hourly rainfall, observed drainage and predicted drainage by NoMP and MP models for the Ontario site, Period 1, peaks $P_{1\text{-}1}^{Ont}$ and $P_{1\text{-}2}^{Ont}$.

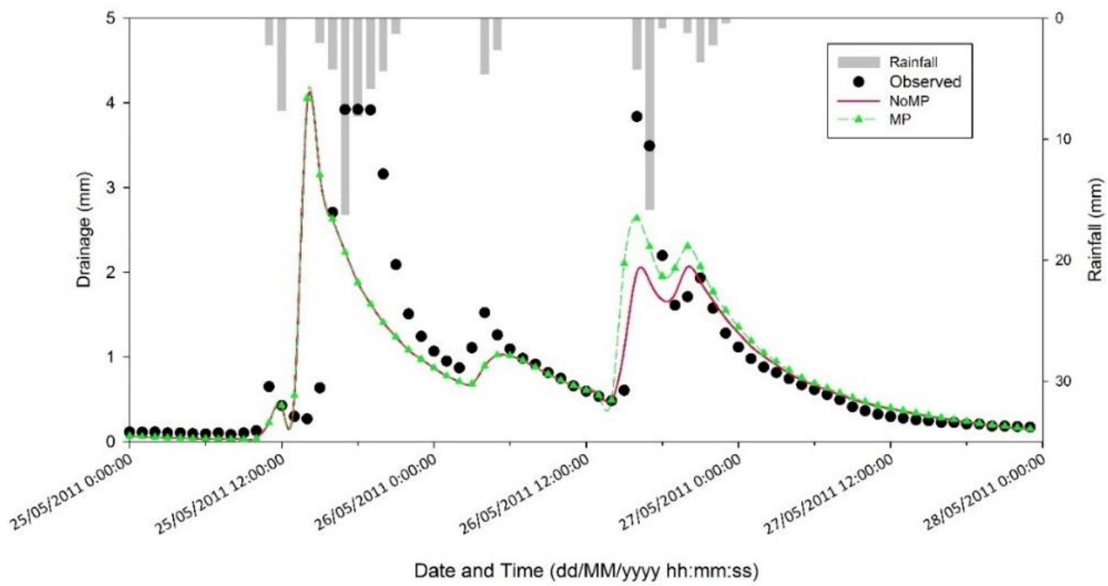

Figure 9. Hourly rainfall, observed drainage and predicted drainage by NoMP and MP models in Ontario, Period 2, peak $P_{2\text{-}1}^{Ont}$. Note that $P_{2\text{-}1}^{Ont}$ is the peak occurring on 26/5/2011 at 16:00

When using hourly data to evaluate short time scale model performance in drainage peak periods, the macropore component significantly improved peak drainage simulations when activated. For the two peaks ($P_{1\text{-}1}^{Ont}$, $P_{1\text{-}2}^{Ont}$) in Period 1 (27-29 June 2008; Table 6), at the Ontario site, the saturated surface soil layer and limited infiltration rate led the two peaks to be seriously underestimated by the NoMP model (PBIAS = 39.97% and 51.59% respectively). When macropores exist, a portion of excess water can penetrate the soil profile and raise drainage peaks. Accordingly, the MP simulation showed PBIAS values of 11.28% and 20.85% for the two peaks (Figure 8, Table 13). Similarly, the PBIAS of the single predicted peak ($P_{2\text{-}1}^{Ont}$) in Period 2 (25th to 27th May, 2011) decreased from 50.69% to 31.35% (Figure 9, Table 13), when the macropore component was activated.

Table 13. Statistics for predicted drainage peak, amount and timing by NoMP and MP in Ontario Period 1, peaks $P_{1\text{-}1}^{Ont}$ *and* $P_{1\text{-}2}^{Ont}$ and Period 2, peak $P_{2\text{-}1}^{Ont}$.

Period	Peak(s)	Model accuracy statistic	Drainage (mm)		
				Simulated	
			Observed	NoMP	MP
Peak value (mm h^{-1})					
1	$P_{1\text{-}1}^{Ont}$		4.583	2.751	4.066
		PBIAS		-39.97%	-11.28%
	$P_{1\text{-}2}^{Ont}$		5.123	2.48	4.055
		PBIAS		-51.59%	-20.85%
2	$P_{2\text{-}1}^{Ont}$		3.837	1.892	2.634
		PBIAS		-50.69%	-31.35%
Cumulated value (mm over Period)					
1	$P_{1\text{-}1}^{Ont} + P_{1\text{-}2}^{Ont}$		27.6	43.2	52.3
		PBIAS		56.52%	89.49%
		NSE		0.48	0.25
		IoA		0.58	0.52
2*	$P_{2\text{-}1}^{Ont}$		78.8	78.2	83.1
		PBIAS		-0.76%	5.46%
		NSE		0.47	0.46
		IoA		0.77	0.75

* includes $P_{2\text{-}1}^{Ont}$ and peak at 18:00 on 25 May 2011.

However, the overall quantity and timing of drain flow simulated with the MP model were not as good as those simulated by the NoMP model. The PBIAS increased from 56.52% to 89.49% in Period 1 (peaks $P_{1\text{-}1}^{Ont} + P_{1\text{-}2}^{Ont}$), and from -0.76% to 5.46% in Period 2 (peak $P_{2\text{-}1}^{Ont}$). There were larger overestimations in MP, because the preferential flow in macropores was quickly drained out, thereby raising the drainage peak; however, the soil matrix was still saturated by vertical infiltration or lateral absorption, and this part of soil water, still driven by equilibrium potentials was drained out with delay into post-peak hours. The measured drainage rate therefore decreased gradually and caused a slow recession (Figure 8, 9), whereas the flat simulated peaks overestimated reality. Accordingly, the NSE and IoA were also lower in MP than NoMP simulations (Table 13).

3.4.2 Comparison between Simulations with and without macropores in Iowa

In the long term scenario at the Iowa site, the effects of the use of the macropore component on simulations were analyzed on daily scale (Figure 10). The predicted drainage from the NoMP and MP models were almost identical except for one high drainage day (*i.e.*, 21 August 2007), which was also the only period during which the macropore component of the model was called upon during this period. Because macropores are not active unless surface runoff occurs, 21 August 2007 was the only day when sufficient simulated runoff occurred for the macropore component to be called upon. In this period of surface runoff, 35.74 mm macropore flow penetrated into the soil, which resulted in a 31.88 mm greater tile drainage volume, as only a small fraction of macropore flow was laterally absorbed by the surrounding soil. Thus, the simulation with the MP model less accurately predicted a 3.7% greater cumulative drainage over the two years than the NoMP model. However, higher drainage rates (peaks) were better simulated by the MP than NoMP model, resulting in the former model’s better performance in predicting drainage pattern, raising the NSE from 0.71 to 0.73, and the IoA from 0.757 to 0.762 (Table 14).

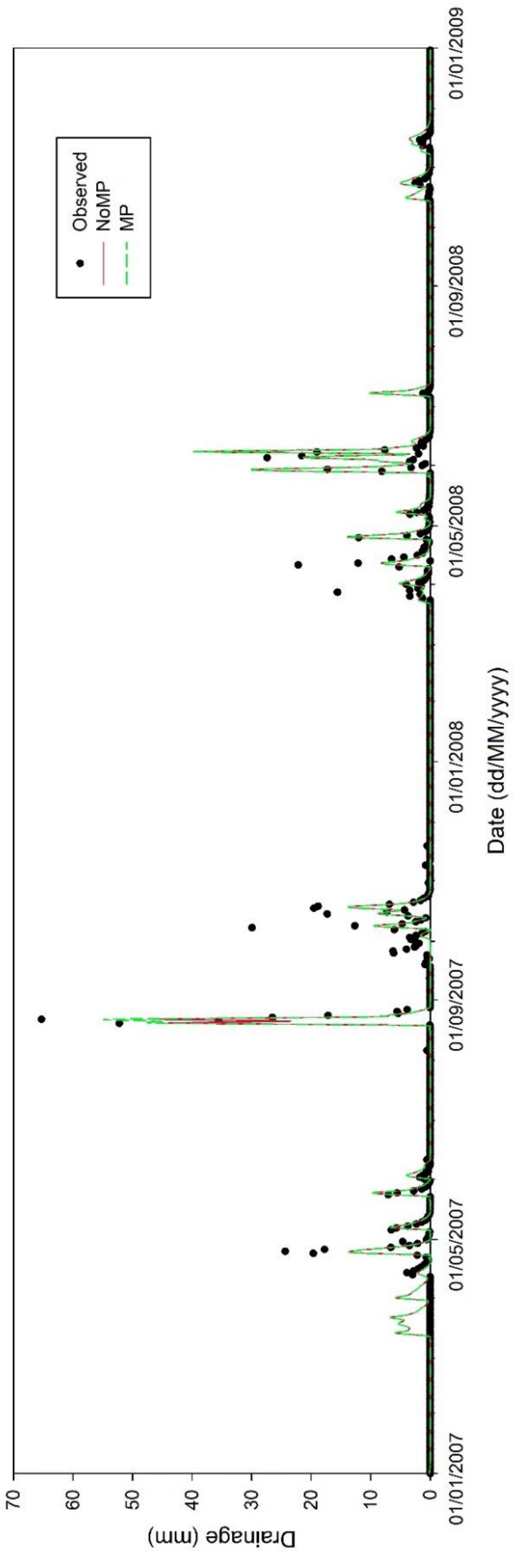

Figure 10. Observed daily drainage flow and predicted daily drainage flow by NoMP and MP at Iowa site.

Table 14. Model accuracy statistics for no macropore (NoMP) and with macropore (MP) RZWQM2 models in long term drainage simulation, Iowa site.

Model accuracy statistic	Cumulated Drainage (mm)		
		Simulated	
	Observed	NoMP	MP
	810.4	862.8	894.9
PBIAS		6.47%	10.43%
NSE		0.71	0.73
IoA		0.757	0.762

Again, with the Iowa data, we analyzed model performance of peak simulation at an hourly scale. Since macropore flow only occurred during one peak period in the whole data set, hourly data for the unique period of August 19th to August 23rd 2007 was used (Figure 11).

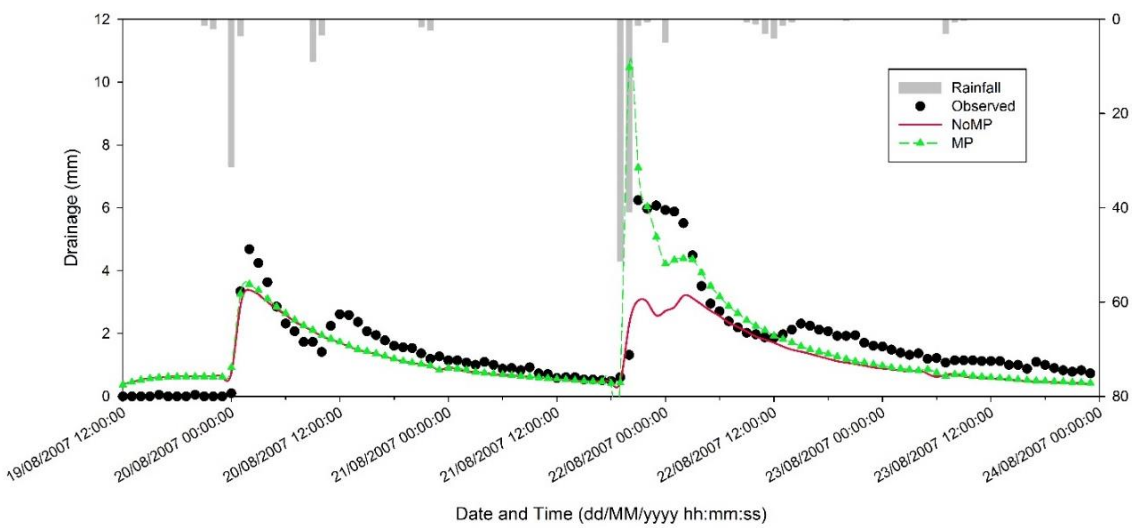

Figure 11. Hourly rainfall, observed drainage and predicted drainage by NoMP and MP models in Iowa, Period 1 (19th August – 23rd August, 2007), peak $P_{1\text{-}1}^{Iowa}$.

Based on hourly results from the Iowa site (Table 15), the MP model raised the simulated peak value, which was seriously underestimated by the NoMP model, and improved the IoA. Due to the preferential flow, the MP model predicted a sharp peak of with 10.46 mm on August 21st after an intensive rainfall, while the NoMP underestimated this peak at only 3 mm. As shown in

Figure 11, In Period 1 in Iowa, the peak showing the greatest difference between two models' simulations was the second one during a continuous rainfall event. The first peak (in early morning of 20th August, 2007) was well simulated, and there was no difference between MP and NoMP, because the simulated (and actual) surface soil layer was capable of allowing all the surface water to infiltrate. When there is no runoff the macropore flow portion of the model is not implemented. However, when the second intensive rainfall event occurred, the wet soil surface blocked out the excess water under the NoMP model, leading to surface runoff, whereas the MP model allowed water to keep penetrating into the soil through macropores, thereby raising the second drainage peak.

Table 15. Statistics for predicted drainage peak, amount and timing by NoMP and MP in Iowa (Peak period: 19th August – 23rd August, 2007).

Period	Peak(s)	Model accuracy statistic	Drainage (mm)		
				Simulated	
			Observed	NoMP	MP
			Peak value (mm h^{-1})		
1	$P_{1\text{-}1}^{Iowa}$		6.24	3.0	10.46
		PBIAS		-51.92%	67.63%
			Cumulated value (mm over Period)		
1	$P_{1\text{-}1}^{Iowa}$		179.5	134.5	166.2
		PBIAS		-25.07%	-7.40%
		NSE		0.54	0.36
		IoA		0.68	0.71

Although the PBIAS for simulated peak values was not substantially improved by using the MP *vs.* NoMP model (PBIAS = 67.63% *vs.* -51.92%, respectively), the cumulated drainage volume for this period was better predicted by the MP *vs.* NoMP model (PBIAS = -7.40% *vs.* -25.07%, IoA = 0.71 *vs.* 0.68, NSE = 0.36 *vs.* 0.54, respectively). Because the NSE value is dependent on the matchups of observed and simulated values in each hour, the result indicated that

NoMP model better simulated the drainage peak timing compared with MP model. As the simulated peak in MP (10.46 mm) occurred one hour earlier than the observed peak, when the observed drainage was low (2.3 mm), this significant difference led to a much lower NSE. The one-hour advance in simulated peak obtained with the MP model could be due to: (i) the macropore flow velocity calculated by the macropore component being faster than it is in reality, or (ii) the measurement bias in one hour.

3.4.3 Sensitivity analysis

Sensitivity tests were conducted to investigate the effects of macroporosity and pore radius on total macropore flow in the simulations and results from the Ontario and Iowa sites were similar (Figure 12, 13). Predicted macropore flow was relatively insensitive to the macropore input parameters, thus, the model's macropore component is not sufficiently sensitive enough to mimic real macropore structure quantitatively. According to the equations in RZWQM2, increasing macroporosity can provide more open channels for surface water to flow through, thereby increasing macropore flow. Conversely, as shown in Eq. 19, a larger pore radius can result in a lesser number of macropores which can accept excess water, and lead to lesser macropore flow in the scenario. Based on results from the Ontario and Iowa scenarios, macropore flow did not monotonously increase or decrease with the changes in macropore parameters. At the Ontario site, reducing macroporosity by 10% - 30% resulted in a 0.5% increase in total macropore flow. Increasing macropore radius by 10%-30% would in theory reduce macropore flow; instead, the flow increased by 0.5%. Similar fluctuations occurred for the Iowa scenario: with a 30% change in this parameter, there was a slight opposite effect on macropore flow.

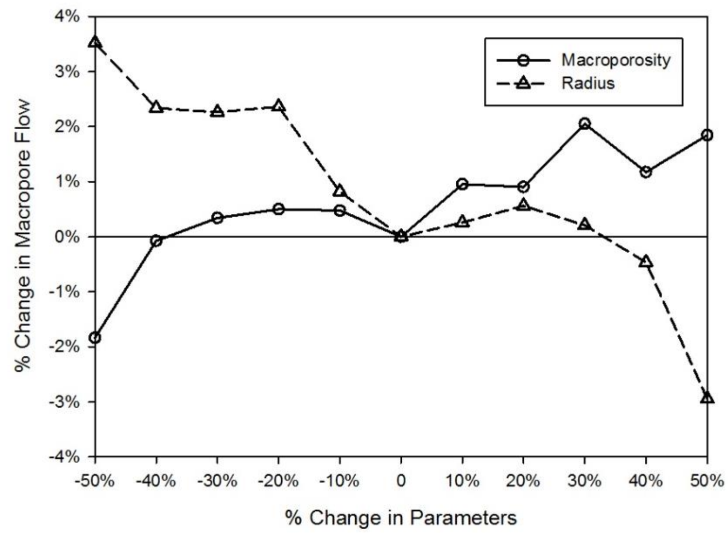

Figure 12. Parameter sensitivity for macropore flow in Ontario scenario.

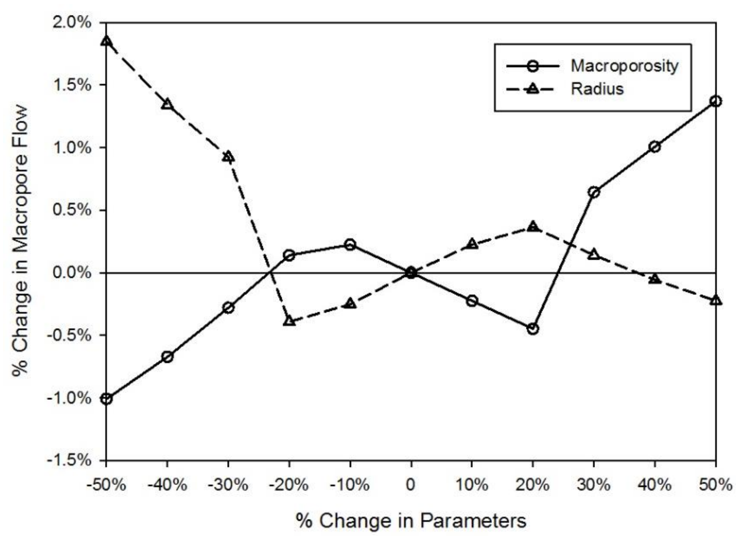

Figure 13. Parameter sensitivity for macropore flow in Iowa scenario.

There are some possible reasons for this unexpected effect:

i. the balance between lateral absorption and vertical macropore flow may be altered. When macroporosity is increased or the radius is decreased, the total number of macropores is increased, thus, there is more lateral absorption by surrounding soils. Conversely, if the change in absorption is greater than the change in water flow, the total macropore flow could be reduced.

ii. changing the parameters might not only result in a different amount of water, but might also alter the velocity of macropore flow. In each time step, the water in macropore channels is routed downward to deeper soil layers, then the lateral absorption rate will depend on the soil moisture deficit in that specific layer. According to Eqs. 20 and 21, macroporosity and pore radius affect the maximum macropore flow capacity, resulting in different depths at which lateral absorption occurs. Therefore, the total macropore flow would be influenced.

iii. since the components in the model are interactive, changing parameters in the macropore component of the model will also affect soil moisture distribution throughout the whole soil matrix. As a result, the plant root uptake, soil surface evaporation and plant transpiration could be altered, and these factors have impact on macropore flow as well.

Although there were fluctuations caused by small changes (within 30%) in parameters, the main effects from macroporosity and radius can still be observed. The fluctuations were always within 0.5% when changes in parameters we <30%; however, when the adjustments in parameters increased to 50%, the main effects of these two parameters became predominant. The changes in macropore flow became larger, ranging from 1% to 4%, and the total amount of flow tended to increase with higher macroporosity, and decrease with larger pore radius. However, overall, total macropore flow was not sensitive to macroporosity and pore radius, a 50% change in parameter only resulting in < 4% change in output.

Sensitivity analysis was also conducted for drainage peak periods on an hourly scale. Results suggest that the main effects of input parameters (macroporosity and radius) on predicted drainage are in the rising limb of the drainage flow hydrograph. We used peaks from the two periods monitored in Ontario and one in Iowa when macropore flow occurred. In each period, parameters ranging from 50% to 150% of the original calibrated values were factorially combined as input for the model, the mean simulated values and the standard errors from the factorial tests were collected (Figure 14). An error bar was displayed on each hourly simulation (±3× standard errors). In most simulations, the ratio of 3× standard error to mean ($R_{3s.e./mean}$) was lower than 1%, which indicated that the variability of simulated drainage was small even when input parameters varied across a relatively larger range (50% to 150%). The most significant effects caused by parameter changes occurred in the peak hours and the rising limb of the tile drainage hydrograph (Figure 14). For Ontario Period 1 (Figure 14-I), the simulated values of two peaks (a, b) showed the greatest variability, with $R_{3s.e./mean}$ of 1.3% and 0.8% respectively, while others were < 0.5%. For the Ontario Period 2 (Figure 14-II), the largest $R_{3s.e./mean}$ also occurred in the peak or rising hours (c, d, e, f), with $R_{3s.e./mean}$ values of 3.9%, 6.1%, 0.8% and 4.1% for the four peaks, respectively. The pattern for the Iowa scenario was similar. The three simulated peaks most affected by parameters (g, h, i) are shown in Figure 14-III; their $R_{3s.e./mean}$ values were 19.36%, 1.9% and 1.3% respectively.

The reason for the effectiveness of macropores during the rising period arises from the fact that preferential flow is faster than water movement in the soil matrix and reaches the water table first. The effects of this flow are shown in an earlier drainage period. However, these effects are not sensitive to the macropore parameters tested, variations in predicted drainage peaks being within 5% when parameters are varied by 50% - 150%. In addition, after the peak hour, drainage is dominated by equilibrium flow, so macropores have little impact in the recession period of the drainage hydrograph. Therefore, there is nearly no variability in simulations during those hours.

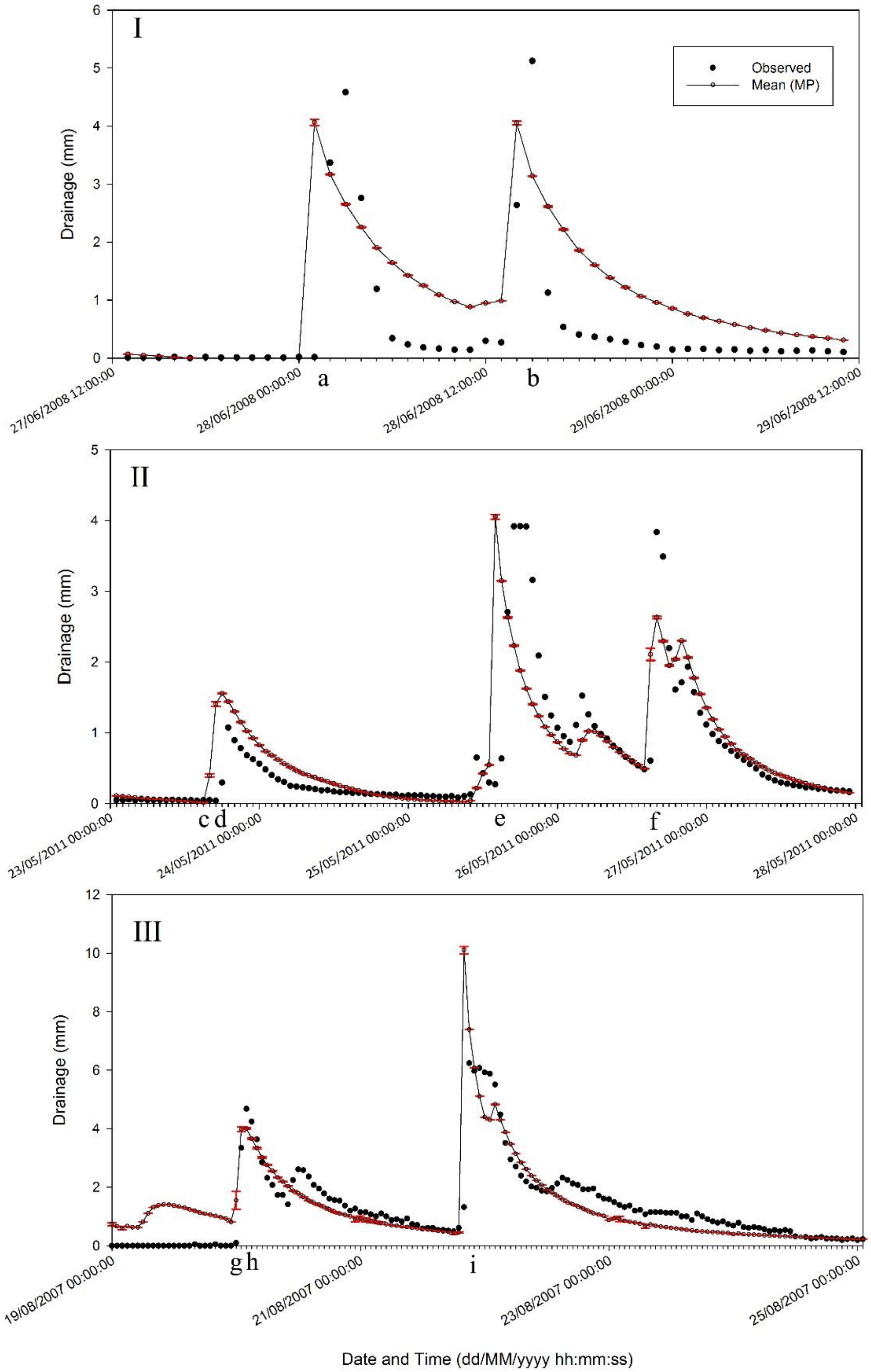

Figure 14. Parameter sensitivity for predicted hourly drainage in three peak periods. (I: Ontario Period 1; II: Ontario Period 2; III: Iowa peak Period 1)

3.5 Summary and Conclusions

This study calibrated the macropore component of RZWQM2 against observed hourly tile drainage data from two drainage sites in Ontario and Iowa. At each site, by comparing the performance of models with and without activating the model's macropore component, we evaluated the overall effects of this component over long term periods, as well as the model's ability to simulate drainage peaks on a precise hourly scale.

Over whole simulation periods (several days), the effects of implementing the macropore component on drainage were not significant. The drainage distribution remained unchanged except for several drainage peak periods during the long term simulation. Considering macropores, there was a 6% increase of predicted drainage volume over the four-year scenario in Ontario, and a 3.7% increase over two-year scenario in Iowa.

When focusing on drainage peak periods at an hourly scale, the macropore component does improve the model performance in catching hourly drainage peaks. These peaks, usually underestimated by the NoMP model, generally occurred during an intensive rainfall event or under condition with a saturated soil surface. In such cases, the predicted peak values were significantly closer to observed values with the MP model, compared with the NoMP model. This implied that activating the macropore component would mimic more closely real field condition, and could solve problems of peak underestimation in RZWQM2. However, in most of the cases total drainage amount and drainage timing predicted by the MP model were worse than those simulated by the NoMP model. The preferential flow is dominant in the raising period of a peak and causes a sharp ascent at the beginning, which is similar to the observations, but in the recession period, the curve is flatter due to the subsequent equilibrium flow, which does not match the observed pattern. As a result, the overall performance in peak simulation is affected.

The sensitivity analysis of the model's macropore component indicated that drainage simulations were rather insensitive to the model's macroporosity and radius parameters. With a 50% change in these calibrated parameters, the changes in total macropore flow were < 4%, and the changes in predicted peak values were < 5%.

In conclusion, activating the macropore component in RZWQM2 can raise predicted drainage peaks which are underestimated by the model without this component, however, the implementing the macropore component results in insensitivity to macroporosity and pore radius, the variability of predicted macropore flow being so small that it cannot be adjusted to cover a wide range by simply adjusting the parameters. Therefore, the calibrated parameters are not sensitive enough to represent real macropore structure or estimate macropore properties quantitatively. Although RZWQM2 has the capability to simulate macropore flow, more study should be conducted to investigate the hydrologic process of preferential flow in macropore channels, and appropriately modify the macropore component of RZWQM2 in order to provide more precise drainage simulations. Future investigations include: 1) develop better soil water movement assumption in macroporous soil and macropore channels to shorten drainage peak recession time, 2) try different drainage simulation approaches to magnify the effects from macropore parameters so that user can calibrate RZWQM2 with high time resolution data, 3) in order to reduce effects from variability of measurements and complicated field condition, the tests on macropore flow simulations can be conducted in undisturbed soil core experiments first.

Chapter 4. Summary and Conclusions

This study evaluated different approaches in improving RZWQM2 performance of drainage peaks simulations, based on hourly scale data from two experiment sites in Iowa and Ontario respectively.

In Chapter 2, the modified RZWQM2 with soil water redistribution and drainage occurring simultaneously with the infiltration of rainfall showed advantages in simulating the timing of drainage peak and drainage pattern, by which it improved overall model performance. This is important to the simulation in the fate and transport of agricultural contaminant in tile drainage water, as the pesticides and herbicides are transported along with soil water. The fate and high concentration leaching issue of contaminants are highly related to subsurface drainage peaks. A better simulation in peak timing leads to a more accurate prediction in contaminants transportation, especially for those with short degradation half-life time. However, no significant difference amongst the three equations was found, and the two transient equations didn’t improve drainage simulation in hourly drainage. This section indicates that, RZWQM2 should be modified to allow soil water redistribution and drainage occur simultaneously with the infiltration of rainfall in order to better simulate the drainage timing. The steady state assumption of original Hooghoudt Equation in RZWQM2 is appropriate with small time step simulations, and it performs satisfactorily in the model.

Chapter 3 evaluated the macropore component of RZWQM2, in order to test the effects of preferential flow on drainage peak simulations and solve the underestimation in drainage peak values in Chapter 2. The results showed that, macropore component could enhance the simulated peak values, which were underestimated or even not simulated at all when macropore was not taken into account. However, the total drainage amount and timing of the periods were not predicted well because of the slow drawdown which was resulted by equilibrium flow in soil matrix. Further, the two parameters, macroporosity and pore radius, were not sensitive in this component, and the variability of predicted macropore flow was negligible even the parameters were adjusted in a relatively larger range. To improve macropore component in RZWQM2, appropriate preferential flow assumptions should be implemented in the model which allow quicker drainage peak recession and make macropores parameters more sensitive.

Here are some recommendations for future studies in relevant field:

1. Other transient state drainage equations based on various assumptions could be tested in RZWQM2 to improve performance, meanwhile, different assumptions in RZWQM2's hydrologic component can be tested. In this study, the soil water redistribution process was improved, while the assumptions of drain tile flow process, water table update and soil water deficit calculation in each soil horizon can also have significant impact on subsurface drainage simulation. More comprehensive improvement could be implemented to RZWQM2.

2. The preferential flow process in macropore channels under real condition should be further investigated. The model performance could be improved by adopting a more appropriate algorithm. For example, a better soil water movement process (vertical penetration and horizontal infiltration) in macroporous soil and macropore channels can lead to shorter drainage peak recession time, which better match observed drainage peak events. In addition, adjustments in macropore flow equations can be made to allow macropore parameters become more sensitive in predicting preferential flow.

3. More hourly data from different experimental sites and conditions should be applied to further test the approaches in this study. It is difficult to conduct simulation and analysis with high variability of hourly drainage data, complicated field condition and changing soil condition, thus the tests of different modeling approaches can be evaluated under lab experiment conditions and be further investigated in various field experiments in the future.

References

Abbott, I. and Parker, C.A., 1980. The occurrence of earthworms in the wheat belt of Western Australia in relation to land use and rainfall. Soil Research, 18(3), pp.343-352.

Ahuja, L., Rojas, K.W. and Hanson, J.D., 2000. Root zone water quality model: modelling management effects on water quality and crop production. Water Resources Publication.

Allaire-Leung, S.E., Gupta, S.C. and Moncrief, J.F., 2000. Water and solute movement in soil as influenced by macropore characteristics: 1. Macropore continuity. Journal of Contaminant Hydrology, 41(3), pp.283-301.

Akhand, N., Madani, A. and Gordon, R., 2003. Application of RZWQM in Predicting Subsurface Drainage under Nova Scotia Conditions. Canadian Water Resources Journal, 28(1), pp.1-19.

Baker, J.L., Campbell, K.L., Johnson, H.P. and Hanway, J.J., 1975. Nitrate, phosphorus, and sulfate in subsurface drainage water. Journal of Environmental Quality, 4(3), pp.406-412.

Baker, J.L. and Johnson, H.P., 1981. Nitrate-nitrogen in tile drainage as affected by fertilization. Journal of Environmental Quality, 10(4), pp.519-522.

Beven, K. and Germann, P., 1982. Macropores and water flow in soils. Water resources research, 18(5), pp.1311-1325.

Beven, K. and Germann, P., 2013. Macropores and water flow in soils revisited. Water Resources Research, 49(6), pp.3071-3092.

Bouma, J. and Wösten, J.H.M., 1979. Flow patterns during extended saturated flow in two, undisturbed swelling clay soils with different macrostructures. Soil Science Society of America Journal, 43(1), pp.16-22.

Bouwer, H. and Van Schilfgaarde, J., 1963. Simplified method of predicting fall of water table in drained land. Transactions of ASAE, 6(4), pp.288-291.

Brewer, R., 1965. Fabric and Mineral Analysis of Soils. Soil Science, 100(1), p.73.

Cambardella, C.A., Moorman, T.B., Jaynes, D.B., Hatfield, J.L., Parkin, T.B., Simpkins, W.W. and Karlen, D.L., 1999. Water quality in Walnut Creek watershed: Nitrate-nitrogen in soils, subsurface drainage water, and shallow groundwater. Journal of Environmental Quality, 28(1), pp.25-34.

Darzi-Naftchally, A., Mirlatifi, S.M. and Asgari, A., 2014. Comparison of steady-and unsteady-state drainage equations for determination of subsurface drain spacing in paddy fields: a case study in Northern Iran. Paddy and water environment, 12(1), pp.103-111.

Everts, C.J. and Kanwar, R.S., 1993. Interpreting tension-infiltrometer data for quantifying soil macropores: Some practical considerations. Transactions of the ASAE, 36(2), pp.423-428.

Fleming, R.J. and Bradshaw, S.H., 1992. Detection of soil macropores using smoke. Canadian Society of Agricultural Engineering. Paper, (92-103).

Fox, G.A., Malone, R., Sabbagh, G.J. and Rojas, K., 2004. Interrelationship of macropores and subsurface drainage for conservative tracer and pesticide transport. Journal of Environmental Quality, 33(6), pp.2281-2289.

Ghane, E., Fausey, N.R., Shedekar, V.S., Piepho, H.P., Shang, Y. and Brown, L.C., 2012. Crop yield evaluation under controlled drainage in Ohio, United States. Journal of Soil and Water Conservation, 67(6), pp.465-473.

Gowda, P.H., Mulla, D.J., Desmond, E.D., Ward, A.D. and Moriasi, D.N., 2012. ADAPT: Model use, calibration, and validation. Transactions of the ASABE, 55(4), pp.1345-1352.

Green, R.D. and Askew, G.P., 1965. Observations on the biological development of macropores in soils of Romney Marsh. European Journal of Soil Science, 16(2), pp.342-344.

Helmers, M.J., Lawlor, P.A., Baker, J.L., Melvin, S.W. and Lemke, D.W., 2005. Temporal subsurface flow patterns from fifteen years in north-central Iowa. ASABE Annual International Meeting Paper No. 05, 2234. St Joseph, MI.

Hewitt, J.S. and Dexter, A.R., 1980. Effects of tillage and stubble management on the structure of a swelling soil. European Journal of Soil Science, 31(2), pp.203-215.

Hu, Y., Feng, J., Yang, T. and Wang, C., 2014. A new method to characterize the spatial structure of soil macropore networks in effects of cultivation using computed tomography. Hydrological Processes, 28(9), pp.3419-3431.

Kanwar, R.S., Colvin, T.S. and Karlen, D.L., 1997. Ridge, moldboard, chisel, and no-till effects on tile water quality beneath two cropping systems. Journal of Production Agriculture, 10(2), pp.227-234.

Kanwar, R.S., Karlen, D.L., Colvin, T.S., Simpkins, W. and McFadden, V.J., 1993. Evaluation of tillage and crop rotation effects on groundwater quality. Completion Report, Leopold Center for Sustainable Agriculture, Iowa State University, Ames, IA, 103p.

Kladivko, E.J., Van Scoyoc, G.E., Monke, E.J., Oates, K.M. and Pask, W., 1991. Pesticide and nutrient movement into subsurface tile drains on a silt loam soil in Indiana. Journal of Environmental Quality, 20(1), pp.264-270.

Kohler, A., Abbaspour, K.C., Fritsch, M., Van Genuchten, M.T. and Schulin, R., 2001. Simulating unsaturated flow and transport in a macroporous soil to tile drains subject to an entrance head: Model development and preliminary evaluation. Journal of Hydrology, 254(1), pp.67-81.

Krysanova, V. and White, M., 2015. Advances in water resources assessment with SWAT—an overview. Hydrological Sciences Journal, 60(5), pp.771-783.

Kumar, A., Kanwar, R.S. and Ahuja, L.R., 1998. Evaluation of preferential flow component of RZWQM in simulating water and atrazine transport to subsurface drains. Transactions of the ASAE, 41(3), pp.627-637.

Kumar, R., Bhakar, S.R., Jhajharia, D. and Morvejalahkami, B., 2012. Evaluation of drain spacing equations in the Indira Gandhi Canal command area, India. ISH Journal of Hydraulic Engineering, 18(3), pp.186-193.

Lawes, J.B., 1882. On the amount and composition of the rain and drainage-waters collected at Rothamsted. Journal of the Royal Agricultural Society of England. Second Series, Volume 17, Part 2, No.34..

Lawlor, P.A., Helmers, M.J., Baker, J.L., Melvin, S.W. and Lemke, D.W., 2008. Nitrogen application rate effect on nitrate-nitrogen concentration and loss in subsurface drainage for a corn-soybean rotation. Transactions of the ASAE, 51(1), p.83.

Liu, H.L., Yang, J.Y., Tan, C.S., Drury, C.F., Reynolds, W.D., Zhang, T.Q., Bai, Y.L., Jin, J., He, P. and Hoogenboom, G., 2011. Simulating water content, crop yield and nitrate-N loss under free and controlled tile drainage with subsurface irrigation using the DSSAT model. Agricultural Water Management, 98(6), pp.1105-1111.

Liu, M.X., Cui, W.H., Wu, D., Liao, L.J. and Du, W.Z., 2014. Soil Macropore structures and their effect on preferential flow. Applied Mechanics and Materials, v522-524 (2014 01 01): 990-994.

Lu C., 2015. Modeling surface runoff and subsurface tile drainage under drainage and controlled drainage with sub-irrigation in southern Ontario[D]. MSc. Thesis. McGill University.

Ma, L., Malone, R.W., Heilman, P., Ahuja, L.R., Meade, T., Saseendran, S.A., Ascough, J.C. and Kanwar, R.S., 2007. Sensitivity of tile drainage flow and crop yield on measured and calibrated soil hydraulic properties. Geoderma, 140(3), pp.284-296.

Ma, L., Malone, R.W., Heilman, P., Karlen, D.L., Kanwar, R.S., Cambardella, C.A., Saseendran, S.A. and Ahuja, L.R., 2007. RZWQM simulation of long-term crop production, water and nitrogen balances in Northeast Iowa. Geoderma, 140(3), pp.247-259.

Malone, R.W., Shipitalo, M.J., Ma, L., Ahuja, L.R. and Rojas, K.W., 2001. Macropore component assessment of the Root Zone Water Quality Model (RZWQM) using no-till soil blocks. Transactions of the ASAE, 44(4), pp.843-852.

Malone, R.W., Ahuja, L.R., Ma, L., Don Wauchope, R., Ma, Q. and Rojas, K.W., 2004. Application of the Root Zone Water Quality Model (RZWQM) to pesticide fate and transport: an overview. Pest Management Science, 60(3), pp.205-221.

Meng, C., Niu, J., Li, X., Luo, Z., Du, X., Du, J., Lin, X. and Yu, X., 2016. Quantifying soil macropore networks in different forest communities using industrial computed tomography in a mountainous area of North China. Journal of Soils and Sediments, pp.1-14.

Mishra, G.C. and Singh, V., 2007. A new drain spacing formula. Hydrological Sciences Journal, 52(2), pp.338-351.

Moriasi, D.N., Gitau, M.W., Pai, N. and Daggupati, P., 2015. Hydrologic and water quality models: Performance measures and evaluation criteria. Transactions of the ASABE, 58(6), pp.1763-1785.

Moriasi, D.N., Gowda, P.H., Arnold, J.G., Mulla, D.J., Ale, S. and Steiner, J.L., 2013. Modeling the impact of nitrogen fertilizer application and tile drain configuration on nitrate leaching using SWAT. Agricultural Water Management, 130, pp.36-43.

Mosley, M.P., 1982. Subsurface flow velocities through selected forest soils, South Island, New Zealand. Journal of Hydrology, 55(1-4), pp.65-92.

Omoti U, Wild A. 1979. Use Of Fluorescent Dyes To Mark The Pathways Of Solute Movement Through Soils Under Leaching Conditions: 2. Field Experiments[J]. Soil Science, 128(2): 98-104.

Oosterbaan, R.J., 1994. Agricultural drainage criteria. International Livestock Research Institute Publication, 16, pp.635-690.

Pali, A.K., Katre, P. and Khalkho, D., 2014. An unsteady subsurface drainage equation incorporating variability of soil drainage properties. Water Resources Management, 28(9), pp.2639-2653.

Péron, H., Hueckel, T., Laloui, L. and Hu, L., 2009. Fundamentals of desiccation cracking of fine-grained soils: experimental characterisation and mechanisms identification. Canadian Geotechnical Journal, 46(10), pp.1177-1201.

Perret, J., Prasher, S.O., Kantzas, A. and Langford, C., 1999. Three-dimensional quantification of macropore networks in undisturbed soil cores. Soil Science Society of America Journal, 63(6), pp.1530-1543.

Qi, Z., Helmers, M.J. and Lawlor, P.A., 2008. Effect of different land covers on nitrate-nitrogen leaching and nitrogen uptake in Iowa. ASABE Annual International Meeting Paper No. 084806. St. Joseph, Mich.

Qi, Z., Helmers, M.J., Malone, R.W. and Thorp, K.R., 2011. Simulating long-term impacts of winter rye cover crop on hydrologic cycling and nitrogen dynamics for a corn-soybean crop system. Transactions of the ASABE, 54(5), pp.1575-1588.

Qi, Z., Singh, R., Helmers, M.J. and Zhou, X., 2015. Evaluating the performance of DRAINMOD using soil hydraulic parameters derived by various methods. Agricultural Water Management, 155, pp.48-52.

Qi, Z., Helmers, M.J., Malone, R.W. and Thorp, K.R., 2011. Simulating long-term impacts of winter rye cover crop on hydrologic cycling and nitrogen dynamics for a corn-soybean crop system. Transactions of the ASABE, 54(5), pp.1575-1588.

Rabalais, N.N., Turner, R.E. and Wiseman, W.J., 2001. Hypoxia in the Gulf of Mexico. Journal of Environmental Quality, 30(2), pp.320-329.

Reeve, M.J., Hall, D.G.M. and Bullock, P., 1980. The effect of soil composition and environmental factors on the shrinkage of some clayey British soils. Journal of Soil Science, 31(3), pp.429-442.

Ritzema, H.P., Satyanarayana, T.V., Raman, S. and Boonstra, J., 2008. Subsurface drainage to combat waterlogging and salinity in irrigated lands in India: Lessons learned in farmers' fields. Agricultural Water Management, 95(3), pp.179-189.

Sands, G.R., Song, I., Busman, L.M. and Hansen, B.J., 2008. The effects of subsurface drainage depth and intensity on nitrate loads in the northern cornbelt. Trans. ASABE, 51(3), pp.937-946.

Fangmeier, D.D., 2006. Soil and water conservation engineering. Clifton Park, NY: Thomson Delmar Learning.

Sharma, D.P. and Gupta, S.K., 2006. Subsurface drainage for reversing degradation of waterlogged saline lands. Land Degradation & Development, 17(6), pp.605-614.

Shokri, A. and Bardsley, W.E., 2014. Enhancement of the hooghoudt drain-spacing equation. Journal of Irrigation and Drainage Engineering, 141(6), p.04014070.

Simard, R.R., Beauchemin, S. and Haygarth, P.M., 2000. Potential for preferential pathways of phosphorus transport. Journal of Environmental Quality, 29(1), pp.97-105.

Singh, K.M., Singh, O.P., Ram, S. and Chauhan, H.S., 1992. Modified steady state drainage equations for transient conditions in subsurface drainage. Agricultural water management, 20(4), pp.329-339.

Singh, P. and Kanwar, R.S., 1995. Modification of RZWQM for simulating subsurface drainage by adding a tile flow component. Transactions-American Society of Agricultural Engineers, 38, pp.489-489.

Singh, R., Helmers, M.J. and Qi, Z., 2006. Calibration and validation of DRAINMOD to design subsurface drainage systems for Iowa's tile landscapes. Agricultural Water Management, 85(3), pp.221-232.

Skaggs, R.W., 1978. A water management model for shallow water table soils. North Carolina. University. Water Resources Research Institute. Report (USA). No: 134.

Skaggs, R. W. 1977. Evaluation of drainage-water table control systems using a water management model. In: (G J Hoffman, ed.) Proc. 3rd Natl. Drainage Symposium, 61-68. ASAE Publication 1-77. St. Joseph, Mich.: ASAE.

Skaggs, R.W., 1982. Field evaluation of a water management simulation model. Transactions of the ASAE, 25(3), pp.666-674.

Skaggs, R.W., Youssef, M.A. and Chescheir, G.M., 2012. DRAINMOD: Model use, calibration, and validation. Transactions of the ASABE, 55(4), pp.1509-1522.

Sogbedji, J.M. and McIsaac, G.F., 2002. Evaluation of the ADAPT model for simulating water outflow from agricultural watersheds with extensive tile drainage. Transactions of the ASAE, 45(3), pp.649-659.

Stamm, C.H., Flühler, H., Gächter, R., Leuenberger, J. and Wunderli, H., 1998. Preferential transport of phosphorus in drained grassland soils. Journal of Environmental Quality, 27(3), pp.515-522.

Stampfli, N. and Madramootoo, C.A., 2006. Water table management: A technology for achieving more crop per drop. Irrigation and Drainage Systems, v20 n1 (200602): 41-55.

Tan, C.S., Zhang, T.Q., Drury, C.F., Welacky, T.W. and Reynolds, W.D., 2009. Impacts of Liquid and Solid Manures under Controlled Drainage with Sub-irrigation Recycling Systems on Water Quality and Crop Production. American Society of Agricultural and Biological Engineers.

Tan, C.S. and Zhang, T.Q., 2011. Surface runoff and sub-surface drainage phosphorus losses under regular free drainage and controlled drainage with sub-irrigation systems in southern Ontario. Canadian Journal of Soil Science, 91(3), pp.349-359.

USDA. 1985. Soil survey of Pocahontas County, Iowa. Washington, D.C.: USDA Soil Conservation Service.

USDA-ARS. 1992. Root Zone Water Quality Model (RZWQM): User’s Manual. GPSR Technical Report No. 3. Ft. Collins, Colo.: USDA-ARS, Great Plains Systems Research Unit.

Van Schilfgaarde, J., 1963. Design of tile drainage for falling water tables. Journal of the Irrigation and Drainage Division, 89(2), pp.1-12.

Wang, X., Mosley, C.T., Frankenberger, J.R. and Kladivko, E.J., 2006. Subsurface drain flow and crop yield predictions for different drain spacings using DRAINMOD. Agricultural Water Management, 79(2), pp.113-136.