DEVELOPMENT AND EVALUATION OF RZWQM2-P: A MODEL FOR PHOSPHORUS MANAGEMENT IN TILE-DRAINED AGRICULTURAL FIELDS

Department of Bioresource Engineering
McGill University, Montreal

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ABSTRACT

A rising environmental concern, phosphorus (P) loss from agricultural fields via surface runoff or sub-surface drainage ends up in freshwater bodies (river, lakes), where it causes widespread algal blooms and water quality degradation. Recent studies suggest that agricultural fields fitted with artificial tile drainage system contribute heavily to these P losses. Simulation models could help to measure and manage the agricultural P losses and inform prudent management decisions to mitigate this problem in a time saving and cost-effective way. Computer simulation models for this purpose are presently lacking, particularly for tile drained agricultural fields. Accordingly, the present study was undertaken to develop a computer simulation model to simulate P loss from a tile drained agricultural field through different hydrological pathways. A state-of-the-art algorithm to simulate the fate and transport of P in tile-drained agricultural systems is proposed, tested and incorporated into the RZWQM2 model, to take advantage of its hydrologic and agricultural management subroutines — thereby yielding the RZWQM2-P model. Structured according to Jones et al., (1984) with updates and modifications prescribed by Vadas, (2014), the RZWQM2-P model features dedicated manure and fertilizer P pools to simulate P dynamics arising from their application. To simulate daily P absorption/desorption among the P pools, a dynamically changing rate factor is applied rather than a constant rate factor. Tile drainage dissolved reactive P (DRP) and particulate bound P (PP) loss are estimated according to Francesconi et al., (2016) and Jarvis et al., (1999), respectively. Losses of DRP and PP through surface runoff are simulated according to Neitsch et al., (2011) and McElroy et al., (1976), respectively.

The RZWQM2-P model's capacity to simulate the DRP and PP loss from an agricultural field through surface runoff and tile drainage was evaluated using two sets of observed P loss and water flow data collected from subsurface-drained fields under a corn-soybean rotation on a clay loam soil in southwestern Ontario, Canada. For both cases, the RZWQM2-P model performed satisfactorily (NSE > 0.50, PBAIS within ±30%, IoA >0.75). A sensitivity analysis of the RZWQM2-P's input parameters was conducted to facilitate the application of the model by users like agricultural managers and environmental stakeholders. The sensitivity analysis found the simulation of RZWQM2-P's P loss depends on many parameters; however, macroporosity was the preeminent parameter in simulation of all form of P losses. The DRP loss through surface runoff was most sensitive to the P extraction coefficient, and PP loss through surface runoff was mainly governed by the parameters of the Universal Soil Loss Equation. Tile flow DRP and PP losses were most sensitive to the plant P uptake distribution parameter and the soil detachability coefficient. The newly developed RZWQM2-P model is a capable tool for the simulation of P losses from an agricultural field, particularly for the tile-drained fields, however, it requires skilled and computationally demanding modelling.

RÉSUMÉ

La préoccupation environnementale croissante quant aux pertes de phosphore des champs agricoles par voie des eaux d'écoulement en surface et de drainage souterrain s'explique parce que ce polluant se rend éventuellement dans un plan d'eau douce (rivière, lac) où il cause une prolifération d'algues nocives et une dégradation de la qualité des eaux. De récentes études donnent à penser que les champs agricoles équipés d'un système de drainage contribuent largement à ces pertes en P. L'utilisation de modèles de simulation permettrait d'évaluer et de gérer les pertes en P d'origine agricole, et d'appuyer des décisions de gestion agricole permettant de mitiger ce problème d'une manière efficace en temps et en coût. Il nous manque présentement un modèle de simulation permettant de telles analyses, particulièrement pour les champs agricoles soumis à un drainage souterrain. La présente étude visa donc à développer un modèle de simulation informatisé permettant de simuler les pertes en P provenant d'un champ agricole équipé de drainage souterrain, par différentes voies de transport hydrologiques. Une nouvelle génération d'algorithme permettant de simuler le sort et le transport du P dans un système de culture équipé d'un système de drainage souterrain est proposée, éprouvé, puis incorporé dans le code du modèle RZWQM2, afin d'exploiter ses sous-programmes hydrologiques et de gestion agricole — créant ainsi le modèle RZWQM2-P. Structuré selon Jones et al., (1984) et mis-à-jour et modifié selon Vadas, (2014), le modèle RZWQM2-P offre des réservoirs de P dédiés au fumier et aux engrais lors de la simulation de la dynamique du P opérant suite à leur application. Afin de mieux simuler l'absorption/désorption journalière du P entre les réservoirs de P, des taux d'échange dynamiques plutôt que constants furent appliqués. Le P dissout réactif dans les drains souterrains (DRP) et le P liés aux particules (PP) furent estimés selon Francesconi et al., (2016) et Jarvis et al., (1999), respectivement. Les pertes en DRP et PP par ruissellement de surface furent simulées selon Neitsch et al., (2011) et McElroy et al., (1976), respectivement.

L'habilité de RZWQM2-P à simuler avec exactitude les pertes en DRP et PP provenant d'un champ agricole par voie de ruissellement de surface et de drainage souterrain fut évalué grâce à deux ensembles de données de pertes en P et de débit d'eau enregistrés dans des champs du sud-ouest de l'Ontario équipés d'un système de drainage souterrain et soumis à une rotation maïs-fève soja sur un loam argileux. Le modèle RZWQM2-P performa de façon satisfaisante pour chacun des sites (NSE > 0.50, |PBAIS| ≤ 30%, IoA > 0.75). Une analyse de sensibilité des paramètres d'entrée de RZWQM2-P fut entreprise afin de faciliter l'application du modèle par les gestionnaires agricoles et acteurs œuvrant dans le domaine de l'environnement. L'analyse de sensibilité indiqua que l'exactitude de RZWQM2-P's en simulant toutes formes de perte de P dépend de plusieurs paramètres, mais en particulier de la macroporosité du sol. La perte de DRP par l'écoulement en surface s'avéra particulièrement sensible au coefficient d'extraction du P, tandis que la perte de PP par cette même voie était principalement sous l'influence des paramètres de l'équation universelle de perte de sol (USLE). La perte de DRP et PP par voie de drainage souterrain s'avéra particulièrement sensible au paramètre de distribution de l'assimilation du phosphore par la plante, et le coefficient de détachabilité du sol. Le modèle RZWQM2-P nouvellement développé est un outil prometteur pour la gestion du P en milieu agricole, particulièrement pour les terres doués d'un système de drainage souterrain. Cependant il nécessite une haute compétence de modélisation et s'avère exigeant en termes de calcul.

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CONTRIBUTION OF AUTHORS

This thesis has been written in manuscript-based format. All the research work related to writing computer programs, model development, model evaluation, analysis of model simulation results to prepare the manuscripts were done by the Ph.D. candidate, Debasis Sadhukhan, under the supervision of Dr. Zhiming Qi. Dr. Zhiming Qi provided guidance and research ideas for model development and evaluation and is a co-author of all the manuscripts (Chapter 3-5). Dr. Liwang Ma provided the source codes of the RZWQM2 model and guided the development of the model and he is also a coauthor of all the manuscripts (Chapter 3-5). The measured data from the field experiments used in this study to evaluate and to perform sensitivity analysis of the model is provided by Dr. C.S. Tan and Dr. T.Q. Zhang and they are co-authors of the Chapter 3-5. Youjia Li, one of the coauthors of chapter 5, shared views on the model auto calibration and assisted in implementing cloud computations. Dr. Allan A. Andales facilitated my visits to USDA and shared scientific viewpoints relating to model development and evaluation, he is a coauthor of the Chapter 3.

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

NOMENCLATURE

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

P	Phosphorus
RZWQM2	Root Zone Water Quality Model Version 2
RZWQM	Root Zone Water Quality Model
RZWQM2-P	Root Zone Water Quality Model Version 2 - Phosphorus
FresOP	Fresh Organic P
StabOP	Stable Organic P
LabP	Labile P
ActIP	Active Inorganic P
StabIP	Stable Inorganic P
AvFertP	Available Fertilizer P
ResFertP	Residual Fertilizer P
DRP	Dissolved Reactive Phosphorus
PP	Particulate Phosphorus
SumP	Summation of Dissolved Reactive Phosphorus and Particulate Phosphorus
TP	Total Phosphorus
PBIAS	Percent bias
NSE	Nash-Sutcliffe model efficiency
IoA	Index of agreement
OBS	Observed
SIM	Simulated
GH	Grain Harvested
ET	Evapotranspiration
ΔS	Soil water change
Pb	Air entry pressure
λ	Pore Size Distribution Index
K_{sat}	Saturated Hydraulic Conductivity
K_{lat}	Lateral Hydraulic Conductivity
ρ	Soil bulk density
OM	Soil organic matter content
θ_{fc}	Volumetric soil moisture content at field capacity
φ	Soil porosity
θwp	Volumetric soil moisture content at permanent wilting point
pH	soil pH
EPIC	Erosion / Productivity Impact Calculator
ADAPT	Agricultural Drainage and Pesticide Transport
APEX	Agricultural Policy/Environmental eXtender
PLEASE	Phosphorus LEAching from Soils to the Environment
SurPhos	Surface Phosphorus and Runoff Model

USLE	Universal soil loss equation
SCS	Soil Conservation Services
TotalDP	Total dissolved Phosphorus
SA	Sensitivity Analysis
GSA	Global Sensitivity Analysis
EE	Elementary Effect
Mac	Macroporosity
EET	Elementary Effect Test
SAFE	Sensitivity Analysis for Everybody
LAI	Leaf area Index
N	Nitrogen
NO_3^-	Nitrate
NH4	Ammonium
CD	Control Drainage
WM	Winter Manure Application
IM	Injected manure application
CM	Conventional management practice
Tsoil	Soil Temperature

CHAPTER 1

INTRODUCTION

1.1 BACKGROUND

Agriculture phosphorus (P) demand is about 80 - 90% of the total P demand globally and the supply of P is heavily dependent on mined rock phosphate, but this is a non-renewable resource becoming increasingly scarce and expensive day by day (Expertanswer, 2010). P is also very crucial for agricultural production to obtain proper crop growth and to maintain a high yield. It is also an established fact that most of the P applied in the agricultural field is lost and very little of it is consumed by the crops for their growth. This lost P from agricultural fields through water and sediment is becoming a serious environmental concern, degrading the quality of water in fresh water bodies such as lakes, rivers and also in the brackish water around the coastal area where rivers meet the sea, causing widespread P pollution, algal blooms, called eutrophication (Guildford and Hecky, 2000). Eutrophication makes the water unsuitable for human consumption and causing adverse health effect for humans, livestock and aquatic fauna who are coming within direct contact of this kind of water (Dawson, 1998). It is estimated that 80% of the P pollution of Lake Champlain's Missisquoi Bay is estimated to have originated from upstream agricultural lands (Hegman et al., 1999). In Quebec about 156 lakes are already polluted by P (> 0.02 ppm of P) in 2007 due to excessive application of fertilizer and manure in agricultural fields around the region (MSSS, 2007). Previously it was of thought that P is lost from agricultural fields mostly through surface runoff during large storm events (Sharpley et al., 1992; Skaggs et al., 1994; Fausey et al., 1995; Sims et al., 1998), but in some recent studies, artificial tile drainage system was identified as a significant pathway of P losses in many agricultural fields (Gentry et al., 2007; Eastman et al., 2010). It is mainly because of artificial drainage lowers water tables faster, increases subsurface water flow and subsequently reduces surface runoff thus tile drainage contributes to majority of stream flow. For example, in Ohio, USA tile drainage contributed 51% of the annual stream flow (King et al., 2014) and while in Ontario (ON), Canada it is 42% (Macrae et al., 2007). Tan and Zhang (2011) found that subsurface tile drainage in a corn-soybean field, ON contributed up to 97% of P lost to waterways. Jamieson et al., (2003) also found that subsurface drainage is 37.1% of total P loads in agricultural field located near Bedford, Quebec. Ruark et al., (2012) identified that tile drainage P load varies from 17% to 41% of the total P loads in Wisconsin, whereas tiles supplied 16% to 58% of total dissolved P loads. Similar results also have been reported from other studies across mid-western US (Gentry et al., 2007) and Europe (Dils and Heathwaite, 1999; Gelbrecht et al., 2005). P concentrations in tile drainage water (0.01 to 8.0 mg/L) generally exceed critical levels for eutrophication (0.02-0.03 mg L^{-1}) (King et al., 2015). Remediation of eutrophication is difficult at river and lake level, while removal of excess P from water by chemical (Surampalli et al., 1995) and biological (Oehmen et al., 2007) means are complex, expensive and time consuming. Also, it can't be removed by wastewater treatment plants as the non-point source nature of agricultural P loss. So, the only prevention technique is to control the quantity of fertilizer/manure application in the agricultural field. Thus, in order to obtain sustainable development in the agricultural sector, it is necessary to apply P in the agricultural field in such a way, so that it will not only maintain the crop yield and but at the same time it will ensure that the P will remain available for the future food production and will prevent P pollution in water bodies. To manage fertilizer/manure application at agricultural field we need to understand the hydrological, physical and bio-chemical processes which are involved in crop P uptake, P movement within the soil profile and soil water, and transportation of P through runoff, tile drainage and sediments. We also need to know the governing parameters and their influence on these processes. To achieve this, it is required to evaluate all agricultural systems and management practices particularly with tile drainage system on an urgent basis. This is a humongous task to do with conventional field experiments. A recent study by Kleinman et al., (2015) regarding the fate and transport of P from tile-drained agricultural fields indicated that computer simulation models are currently one of the top priorities in improving one's understanding of P dynamics of arable lands in an efficient way. The computer simulation models are useful in assessing and simulating complex hydrological and physiological processes occurring in agricultural fields which would otherwise be costly and can't be physically measured (Vadas et al., 2013), thus allowing more detailed and efficient investigations than conventional field studies. However, current P computer simulation models lack the capacity to adequately simulate P losses from agricultural field, particularly those occurring through tile drainage (Radcliffe et al., 2015). Hence, suitably developed computer-based simulation models are of urgent need to assist agro-environmental managers to manage P as a nutrient as well as a pollutant.

Modelling P dynamics in an agricultural field involves, modelling of the hydrological processes that are occurring on and below the ground surface and of the effects of agricultural management practices. A P model needs to simulate both surface hydrological processes (*e.g.*, soil evaporation, plant transpiration, runoff, and soil erosion), and subsurface hydrological processes (*e.g.*, infiltration, matrix flow, preferential flow or macropore flow, flow to tile drainage, fluctuation of water tables, root water and nutrient uptake, and soil moisture redistribution). Agricultural management practices such as surface irrigation and sub-irrigation, drainage, fertilization, tillage and residue management, and crop rotation influence the fate and transport of P. The success of a P model greatly depends on how effectively and efficiently the model captures these hydrological processes and how these processes are parameterized within the model. The Root Zone Water

Quality Model (RZWQM2, Ahuja et al., 2000) is a field scale agricultural system model and that has been extensively evaluated in assessing the impact of agricultural management practices and climate change on hydrology, water quality, and crop production at locations across the United States (Fang et al., 2014b; Gillette et al., 2018; Hanson et al., 1999; Ma et al., 2007a,b, 2004; Malone et al., 2014; Qi et al., 2011, 2013; Thorp et al., 2007; Wang et al., 2015) and in Canada (Ahmed et al., 2007a,b; Al-Abed et al., 1997; Madani et al., 2002; Jiang et al., 2018). But as of today, RZWQM2 does not have the capability to simulate P fate and transport from agricultural field. Hence, in this study it has been focused to develop a process-based P management model and subsequently incorporate it within the RZWQM2 model as it is equipped with proven subroutines to simulate all the hydrological processes and agricultural management practices required to simulate P dynamics in an agricultural field. The newly developed P model integrated into RZWQM2 model serves as a single tool known as RZWQM2-P model. The RZWQM2-P model is an all-in-one agricultural P simulation model and it addresses the limitations of the present P simulation models as highlighted by Radcliff et al., (2015). The developed RZWQM2-P model has advance capabilities to simulate the P dynamics due to manure and fertilizer applications while special attention was given in simulating P losses (DRP and PP) particularly through tile drainage system.

Simulation of P loss from agricultural fields through surface runoff and tile drainage is an extremely complex phenomenon involving soil physical, chemical, biological and hydrological processes occurring on and below the soil surface. The P simulation by the RZWQM2-P model greatly depends on how effectively and efficiently these processes are calibrated by the model users. There being many input parameters governing P-loss processes, RZWQM2-P is difficult and time-consuming to calibrate. So, a sensitivity analysis is employed to identify influential model parameters so that calibration process is only focused on them to simplify the modelling process.

1.2 OBJECTIVES

The overall goal of this research is to improve one's understanding of the science behind the fate and transport of P from an agricultural field through computer simulation and modelling approach, in order to enable agro-environmental mangers an economic, time saving, and scientific evaluation of agricultural management practices that may mitigate P pollution of freshwater bodies, arising due to the application of fertilizer/manure in agricultural fields. The goal was achieved through the following specific objectives:

1. To develop a computer model to simulate P loss through different hydrological pathways from an agricultural field, based on the most recent scientific findings regarding the fate and transport of P.
2. To incorporate the developed P model into the RZWQM2 model.
3. To test, calibrate and validate the newly developed RZWQM2-P model in simulating P losses in tile drained field under North American conditions.
4. To perform a sensitivity analysis of the developed RZWQM2-P model in order to identify the most sensitive parameters of the model in relation to P simulation.

1.3 THESIS OUTLINE

This thesis has been written in a "manuscript based" style. Chapter 1 is general introduction, which presents the backgrounds, justifications, and objectives of the research. Chapter 2 presents the literature review on some P simulation models and RZWQM2's evaluation and applications under diverse agrarian scenarios. Chapter 3, 4 and 5 present the results of model development, evaluations, applications and sensitivity analysis three research papers with connecting text. Figures and tables are all presented within the texts when it appears for the very first time. The governing equations of the developed P model is presented in Appendix A. All the references cited in the thesis are given at the end of the thesis.

CONNECTING TEXT TO CHAPTER 2

Chapter 1 introduced the background and the objectives of this study. It also pointed out that the presently available P simulation models have limited capacity to simulate P losses particularly from a tile drained agricultural field, while the RZWQM2 model can be used as a basis for the development of a new P simulation model. In the Chapter 2, review of some available P models is presented to highlight their limitations. Besides, a summery of the RZWQM2's key hydrological processes influencing P dynamics along with it's application and evaluation in diverse agrarian scenarios are presented to substantiate the feasibility of the RZWQM2 model to serve as a basis for the development of a new P simulation model for agricultural fields.

CHAPTER 2

LITERATURE REVIEW

Agricultural fields, particularly those with artificial subsurface tile drainage systems, represent a major source of phosphorus (P) reaching surface waters and causing widespread eutrophication. Despite extensive research, significant problems with the nonpoint source pollution of surface waters by agricultural P remain. Presenting a review of present P simulation models and their capacity and limitations in simulating P loss from agricultural fields, particularly through subsurface tile drains, this chapter also summarizes the overall hydrological processes influencing P loss (*e.g.*, runoff, tile drainage, macropore flow etc.), P fate and transport in soil, P transport through tile drains. The P simulation models for agricultural fields reviewed in this chapter include: EPIC (Erosion/Productivity Impact Calculator; Sharpley and Williams 1990), ADAPT (Agricultural Drainage and Pesticide Transport; Chung et al., 1992), APEX (Agricultural Policy/Environmental eXtender; Francesconi et al., 2014), HYDRUS (Boivin et al., 2006, Šimůnek et al., 2008), PLEASE (Phosphorus LEAching from Soils to the Environment; Schoumans et al., 2013), SurPhos (Surface Phosphorus and Runoff Model; Vadas, 2014) and ICECREAM (Tattari et al., 2001). The RZWQM2 model was chosen as a basis for the development of a new P model addressing the limitation of the present model; accordingly, a review of the key hydrological processes of the RZWQM2 model influencing P dynamics and the application and evaluation of the model for diverse agrarian scenarios are presented to substantiate the practicability of using the RZWQM2 model for this purpose.

2.1 P MODELS

Since late 1970s, P simulation models serving as management tools for agricultural fields and tended to be physically or empirically based and driven by climate variables. Since then, despite much progress in the science behind the fate and transport of agricultural P and in the development of P-simulation models, P models available today remain limited in their applicability to predict P losses from agricultural fields, particularly those which are artificially drained (Radcliff et al., 2015). In the following sections, some of the available P models have been reviewed briefly to highlight their strengths and limitations.

2.1.1 EPIC

Based on an algorithm proposed by Jones et al., (1984), the EPIC model's nutrient sub-model is designed to simulate P loss from agricultural fields. The EPIC model has served as the precursor of many other P simulation models. The model divides soil P into five pools (labile, active inorganic, and stable inorganic and fresh and stable organic). Inorganic fertilizer P inputs are added into the labile P pool, whereas, for organic fertilizer, organic fractions and manure are added into the fresh organic P pool, while the inorganic fraction is added into labile P pool. Continuous movement (*e.g.*, mineralization, immobilization, absorption, desorption) of P happens of among these P pools to maintain an equilibrium. The EPIC model's runoff sub model simulates surface runoff volumes and peak runoff rates, given daily rainfall amounts. Runoff volume is estimated by a modified Soil Conservation Service (SCS) curve number technique. Drainage via subsurface drainage systems is treated as a modification of the natural lateral subsurface flow. The EPIC model does not compute the macropore flow process. The model provides options for agricultural management practices. The model is capable of simulating DRP loss both through surface runoff, and tile drainage, while PP loss is only simulated through surface runoff. Using EPIC to conduct a simulation of crop yield, surface runoff, tile drainage and P loss (DRP) from a clay loam soil in Canada's Lake Erie region, Wang et al., (2018a) found the model to simulate crop yields and flow volumes well, but DRP losses only adequately (NSE ~ 0.50). The absence of a preferential flow simulation and the use of a constant coefficient to regulate P flux among the P pools during the model's simulation of phosphorus sorption/adsorption were deemed to be the model's main limitations in simulating P losses.

2.1.2 APEX

Derived from the EPIC model and following the P routines of Jones et al., (1984), the APEX model is a field-scale to small-watershed-scale process-based hydrological model, wherein tile drainage is regarded as a modification of natural lateral subsurface flow of the soil layer bearing the tile. Storage routing theory and pipe flow simulation are used for subsurface flow simulation. The SCS curve number approach is followed as the key method for simulating surface runoff, with infiltration computed as the difference between effective precipitation and surface runoff. The model also includes an option to compute infiltration and runoff by the Green and Ampt (1911) method. Percolation of water through the soil profile is estimated through a cascade approach. However, APEX does not address the macropore flow process. While APEX provides extensive options to simulate different agricultural management practices, it is only capable of simulating of soluble P loss (DRP) transportation through both surface runoff and tile drainage. Drawing on data from a monitored corn-soybean rotation field situated in Michigan's St. Joseph River watershed, Francesconi et al., (2016) evaluated the APEX model's ability to simulate surface and tile DRP transport with its newly incorporated nonlinear (Langmuir) P sorption option. This was added to better simulate P dynamics than the model's earlier user-defined linear P sorption (based on GLEAMS) option. Although the model's overall performance in predicting soluble P was very poor, the inclusion of the Langmuir isotherm improved soluble P sorption estimates in surface runoff and tile drainage during the corn year, when the only P inputs were added. The linear method proved more appropriate during the soybean year when no fertilizers were applied. They suggested further improvements of in the model’s P partitioning processes and the addition of a preferential flow component.

2.1.3 ADAPT

Mainly derived from the GLEAMS (Leonard et al., 1987; Knisel, 1993) and DRAINMOD (Skaggs, 1978, 1982**)** models, ADAPT was mainly enhanced by adding tile drainage, snowmelt, and macropore flow components. The ADAPT model’s P sub-model originated from the EPIC model’s nutrient components. The ADAPT model employs two algorithms for tile drainage simulation: Hooghoudt’s steady state equation (Bouwer and Schilfgaarde, 1963) when the water table’s midpoint rests between the drains the soil surface, and Kirkham’s equation (Kirkham, 1957) when the water table is above the soil surface. Surface runoff is estimated using the SCS curve number method. ADAPT uses a basic approach to computing macropore flow volume, making it a function of clay content and the number of dry days during which the soil water supply has not met the potential evapotranspiration demand. Capable of simulating P losses (DRP) through surface runoff and tile drainage, ADAPT is incapable of modeling PP loss. Its use not being widely reported to date, we are not aware of any direct study of P loss using ADAPT. In a review article Radcliff et al., (2015) stated that “ADAPT is not capable of modeling P fate and transport in drained agro-ecosystems and is unlikely to accurately predict P losses from drained agricultural fields. The model requires improvement to adequately represent the subsurface movement of P as influenced by soil type, farming practices, and drainage water management”.

2.1.4 HYDRUS

A process-based model for simulating movement of water, heat, and multiple solutes in variably saturated media, HYDRUS exists in multiple versions: a one-dimensional version freely available to the public (HYDRUS-1D), and commercial two- and three-dimensional versions (HYDRUS-2D/3D. Providing limited options to simulate agricultural management practices, the HYDRUS model simulates water quality using its solutes module, a general simulation that lacks detailed phosphorus components. HYDRUS adopts two analytical solutions — Hooghoudt's steady state equation (Bouwer and Schilfgaarde, 1963) and Ernst's equation (Ernst, 1962) — for tile drainage simulation and uses numerical solutions to the Richards (1931) equation for infiltration and water movement through the soil profile. Rainfall in excess of the infiltration capacity is diverted as surface runoff. The HYDRUS model's macropore model is complex and offers three modelling options: one dual-porosity model and two dual-permeability models. While HYDRUS is not specifically designed to model P, it can be represented through the model's tile bound solute transport simulations. Accordingly, the HYDRUS model is only capable of simulate P losses (DRP, PP) through tile drainage while P losses through surface runoff cannot be simulated under the current model versions. Using HYDRUS-2D/3D to simulate the fate of phosphorus in a tile-drained clay loam soil located in southern Ontario, Qiao (2013) found the model to perform well on a weekly scale, but poorly on a daily scale. The worse simulation errors happened during the winter period. HYDRUS could be used to simulate P loss in artificially drained fields, however, due to complex macropore flow simulation and the absence of specific P routines, surface runoff and erosion modeling , or extensive agricultural management options, it cannot be effectively used to model P loss from agricultural fields.

2.1.5 PLEASE

A process-based field scale model based on the STONE model (Wolf et al., 2005), PLEASE (Schoumans et al., 2013) was developed to estimate annual nutrient losses from agricultural fields in the Netherlands. PLEASE calculates P loss through tile drainage by multiplying the mean P concentrations in soil layers as a function of depth and the total annual horizontal water flux (Schoumans et al., 2013). The dissolved inorganic P concentration in the soil solution in each layer is calculated using the Langmuir isotherm equation (Van der Zee and Bolt, 1991), whereas the annual horizontal drainage flux is calculated based on effective annual precipitation, water table depth, drainage resistance and depth of two drainage systems (Van der Salm et al., 2011). There is no component within the model to simulate surface runoff and macropore flow and the model is only capable of simulating soluble P loss (DRP) through tile drainage. The model provides limited options to simulate different agricultural management practices and drainage simulation is indirect being mimicked by specifying alternative input parameters for the model (Dupas and van der Salm, 2010). Applied and evaluated in Nordic countries (mostly Denmark) and the Netherlands, the model generally performed well in simulating water quantity in tile drains, except under heavy clay soil conditions. This was probably the result of the absence of a macropore simulation component (Van der Salm et al., 2011). Accordingly, PLEASE only provides annual estimates of the P loss, making it unsuitable for many applications where higher temporal resolution is required. Moreover, PLEASE's lack of components for simulating surface runoff, macropore flow and its limited agricultural management options, further limits its applicability to a wide range of purposes.

2.1.6 SurPhos

A daily-scale empirical P simulation model designed to simulate edge-of-field DRP loss through surface runoff, SurPhos (Vadas, 2014) was developed to be seamlessly integrated into other models to enhance their P simulating ability, particularly with respect to DRP loss through surface runoff subsequent to the application of inorganic fertilizer and manure (Vadas et al., 2007, 2008). The model's basic structure follows that of the EPIC model, with three inorganic P pools (Jones et al., 1984) and four additional manure P pools to simulate manure P dynamics and two additional fertilizer P pools to simulate fertilizer P dynamics. The model adopts an advanced daily absorption/desorption among the inorganic P pools by using a dynamically changing rate factor (Vadas et al., 2006). The model simulates DRP loss in runoff, but neither considers runoff loss of sediment bound P, or subsurface loss of P through leaching or artificial drainage. The model does not have any component to simulate runoff, drainage or macropore flow and requires to be relevant data from other models to simulate P loss. The model's application to agricultural management practices is limited to tillage. In a recent study focusing on the application and evaluation of SurPhos, Wang et al., (2018b) reported the model's performance to be acceptable in simulating soil labile P dynamics, as well as DRP loss in surface runoff for both solid and liquid cattle manure application, as well as inorganic fertilizer application. In comparing SurPhos's performance to that of SWAT in predicting manure phosphorus loss, Sen et al., (2012) opined that the "SWAT-P model should be replaced by the SurPhos model". Although the SurPhos model is a powerful tool to simulate DRP loss through surface runoff, it lacks the self-sufficiency to simulate PP loss through surface runoff and bound P loss though drainage tiles. Moreover due to the absence of surface runoff and macropore flow simulation and the lack of extensive agricultural management options, it cannot be successfully used as a stand-alone model to simulate P loss from agricultural fields.

2.1.7 ICECREAM

The ICECREAM model (Tattari et al., 2001) is an agricultural nutrient management process control model mainly used for simulating P losses through runoff and leaching from agricultural land. Combining the CREAMS (Knisel, 1980) and GLEAMS (Leonard et al., 1987; Knisel, 1993) models, ICECREAM was initially developed to suit conditions in Nordic countries, and further improved by Larsson et al., (2007), who added a macropore flow component. The P component in ICECREAM is based on the P model formerly developed for the EPIC model (Jones et al., 1984), which employs five P pools: the fresh organic P pool, the slowly mineralizable stable organic P pool, the plant available labile P pool, the long-term stable inorganic P pool and the active P pool. The model simulates surface runoff and infiltration into the soil by partitioning precipitation according to the Soil Conservation Service (SCS) Curve Number method. While ICECREAM does not have a water table-based tile drainage component, it uses the summation of matrix and macropore flow flux at tile depth to mimic tile drainage. ICECREAM adopts simple storage routing concepts to simulate matrix flow within the soil profile, while macropore flow is simulated using the dual porosity approach of Larsson et al., (2007). In its present form, ICECREAM can simulate DRP and PP losses through both surface runoff and tile drainage. Widely tested in Sweden by researchers at the Swedish University of Agricultural Sciences, Uppsala to assess its performance in simulating PP and DRP loss through surface runoff, matrix flow and macropore flow (Larsson et al., 2007; Blombäck and Persson, 2009; Liu et al., 2012), the model has also been applied to estimate P losses from agricultural lands for environmental reporting in Sweden and in the European Union (Johnsson et al., 2008) and served to estimate P losses for climate change scenarios in central Sweden’s Svärtaån catchment (Blombäck et al., 2012). The very first ever evaluation of the ICECREAM model outside Nordic countries (Qi et al., 2017) highlighted the model's limited ability to simulate PP loss through tile drainage at a site in Canada. While ICECREAM seems to be the most accurate agricultural P management model in simulating P losses through tile drains from agricultural fields (Radcliffe et al., 2015), it lacks a water table-based tile drainage component, rather adopting simple storage routing concepts to simulate matrix flow within the soil profile. This can be improved by adopting the soil-matric-potential-based Richards equation to simulate matrix flow and Hooghout's equation to simulate tile drainage. ICECREAM's simulation of manure and fertilizer P dynamics appears to be weak as it assumes that manure and fertilizer P are instantaneously mixed into the soil upon application and that there are not separate P pools to simulate manure and fertilizer P dynamics. ICECREAM also computes the daily absorption/desorption of P among the inorganic P pool using a constant rate factor, which can be further improved by adopting a dynamically changing rate factor (Vadas et al., 2006).

2.2 RZWQM2

2.2.1 Model Description

RZWQM2 is a one-dimensional agricultural systems model, developed by USDA–Agricultural Research Service scientists in the mid-1980s and its first version was officially released back in 1992. Subsequently with time, the model underwent many development and modification to improve its capability by many researchers and scientists. The model simulates the interactions and impacts of various agricultural management practices and associated hydrological processes on crop growth, nutrient transformations, and pesticide transport (Ahuja et al., 2000). The model facilitates the simulation of a broad variety of agricultural management practices and scenarios. These management practices include different types of tillage, different methods and timing of fertilizer, manure and pesticide applications, different methods and timings of irrigation, tile drainage and different crop planting methods. Tillage and residue management have an impact on soil physical and hydraulic properties, micro-topography and surface roughness, energy and water balance, and nutrient transfer from soil to surface runoff. Tillage-induced changes to soil hydraulic properties are slowly changed back to their original conditions as rainfall reconsolidates the tilled layers. The model's input data requirements include site-specific weather information (precipitation, minimum and maximum daily air temperature, solar radiation, relative humidity, and wind speed), initial soil nutrient and hydraulic properties, crop cultivar information and field management information. All the processes within the RZWQM2 model runs on daily time steps except the hydrological processes (Figure 2.1), which runs on hourly time steps. A flowchart of the model's operations is presented in Figure 2.2.

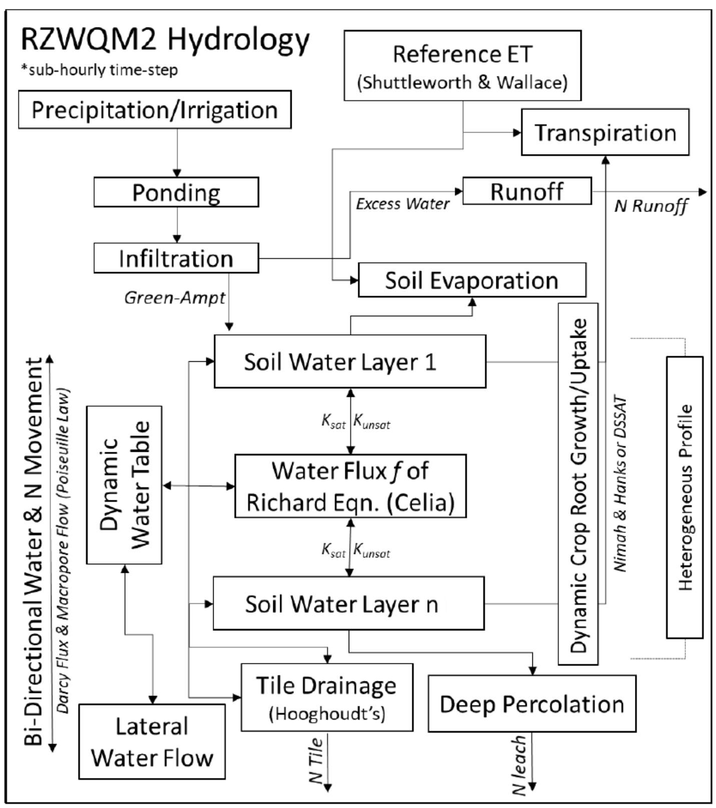

Figure 2.1: Schematic of hydrological processes in RZWQM2 (adopted from Smith, (2019) *)

* permission obtained from the author.

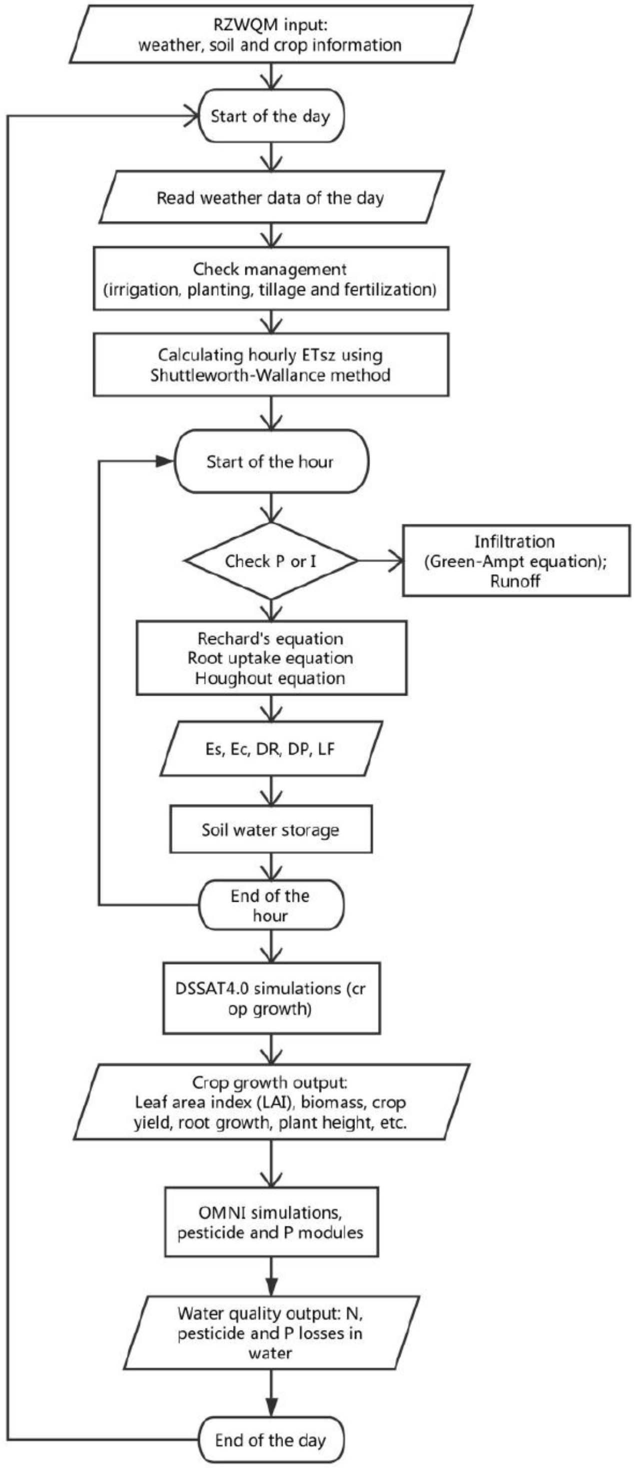

Figure 2.2. Workflow of RZWQM2 (adapted from Fang et al., 2014b *)

E_s is soil water evaporation; E_c is crop transpiration; DP is deep seepage; DR is drainage; LF is lateral flow; P is precipitation; and I is irrigation.

* permission obtained licence no: 486483031565

2.2.2 Hydrological Components

The RZWQM2 model computes the soil water balance as:

$$I + P = ET + R + D + LF + DP \pm \Delta SW \tag{2.1}$$

where, D is tile drainage (mm), DP is deep seepage (mm), ET is evapotranspiration (mm), I is irrigation (mm), LF is lateral flow (mm), P is precipitation (mm), R is runoff (mm), and ΔSW is the change of soil water storage (mm).

Evapotranspiration is estimated using the double layer Shuttleworth-Wallace model (Shuttleworth and Wallace, 1985), while the Richards equation (Eq 2.2) (Richards, 1931) served to simulate soil water redistribution within the soil profile following infiltration of the rainfall and/or irrigation water.

$$\frac{d\theta}{dz} = \frac{d}{dz}\left[K(h,z)\frac{dh}{dz} - K(h,z)\right] - S(z,t) \tag{2.2}$$

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

The infiltration is simulated by the Green-Ampt method (Green and Ampt, 1911).

$$V = K_s \frac{\tau_c + H_0 + Z_{wf}}{Z_{wf}} \tag{2.3}$$

where, H_0 is the depth of surface ponding (mm), if any, K_s is the effective average saturated hydraulic conductivity of the wetting zone (mm s^{-1}), V is the infiltration rate at any given time (mm s^{-1}), Z_{wf} is the depth of the wetting front (mm), and τ_c is the capillary drive or suction head at the wetting front (mm). The soil water content matric suction relationship and unsaturated hydraulic conductivity-matric suction relationships were described by the modified Brooks-Corey relationships (Brooks and Corey, 1964). Surface runoff is generated when the rainfall rate exceeds the infiltration rate. Tile drainage flow is calculated by Hooghoudt's steady state equation (Bouwer and Schilfgaarde, 1963)

$$D = 4.0\ K_e E_m [\frac{2.0 H_d +\ E_m}{S^2}] \tag{2.4}$$

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

Macropores provides a rapid delivery water to tile drains. The simulation of the macropore flow with the RZWQM2 model is governed by Poiseuille's law, assuming gravity flow (Ahuja et al., 2000):

For cylindrical macropores:

$$K_{mac} = \frac{N_p \rho g \pi r_p^4}{8\eta} \tag{2.5}$$

For planar macropores:

$$K_{mac} = \frac{L_c \rho g \pi d^3}{12\eta} \tag{2.6}$$

where, g is the gravitational constant, r_p is the radius of cylindrical holes (cm), L_c is the total length of cracks per unit area (cm), N_p is the number of pores per unit area, η is the dynamic viscosity of water, and ρ is the density of water,

2.2.3 Model Evaluation and Applications

Since the RZWQM2 offers practical options to simulate different agronomic management practices, it had been exhaustively evaluated for its ability to simulate the impacts of agricultural management practices (*e.g*., tile drainage, manure and fertilizer application, pesticide application, water table management, tillage management and cropping system management) and of climate changes on hydrology, water quality (N), and crop growth at locations across the United States (Ma et al., 2007a,b, 2004; Qi et al., 2013, 2011; Wang et al., 2015) and in China (Fang et al., 2010, 2013). A review of studies demonstrating RZWQM2's strengths RZWQM2 in simulating different agricultural management practices follows.

2.2.3.1 Tile Drainage

In most studies the RZWQM2 model's capacity to accurately simulate tile flow and attending nitrogen losses was deemed satisfactory. In the first ever evaluation of the model's capacity to simulate agricultural drainage, Singh and Kanwar (1995a) successfully calibrated and validated the model using measured subsurface drainage flow data compiled under four different tillage treatments implemented at the NERC water quality research site at Nashua, Iowa. They concluded that the model was capable of satisfactorily simulating tile drainage under different tillage practices as its output closely followed the trends of the measured data. Singh and Kanwar (1995b) applied the model to evaluate the impact of different tillage practices on N concentration in soil and N losses in drainage water at the same site as that of their earlier study. This time, the model proved capable of estimating N concentrations in drainage water during the simulated years but failed in calculating the effects of tillage on N losses through tile drainage. In a further study at a field in the Walnut Creek watershed, IA, USA, Bakhsh et al., (2004) showed that RZWQM2-simulated drainage and nitrogen loss through drainage water was comparable to measured data

(Nash-Sutcliffe coefficient (NSE) values of 0.99 and 0.80 respectively). In Canada's coastal areas in Nova Scotia, Akhand et al., (2003) evaluated the performance of RZWQM2 for simulating subsurface drainage flow in a shallow drained soil. Simulated tile drainage agreed closely with measured values with r^2 of 0.60 and 0.57, respectively, for the model calibration and validation phase, indicating the wide adaptability of the RZWQM2 model for subsurface drainage simulation under various climatic and soil conditions. Qi et al., (2011) applied the RZWQM2 model in Iowa, USA to study the long-term (1970-2009) effects on the hydrologic and nitrogen cycles attributable to winter cover crops within a corn-soybean rotation. Daily and annual drainage and annual NO_3^--N loss through tile drainage were satisfactorily simulated by the model, with Nash-Sutcliffe efficiency (NSE) >0.50, ratio of RMSE to standard error (RSR) < 0.70, and percent bias (PBIAS) within ±25% except for the overestimation of annual drainage and NO_3^--N for one treatment. In another study at Iowa, USA, Qi et al., (2012) also reported that the RZWQM2 model performed satisfactorily in simulating of NO_3^--N concentration ([NO_3^--N]) in subsurface drainage under different N fertilizer rates with NSE and PBAIS values of 0.76 and -3%, respectively. Using hourly tile drainage data from Ontario, Canada, and Iowa, USA, Xian et al., (2017) reported that the hourly simulation of tile drainage could be enhanced by enabling the macropore component of RZWQM2. All these studies established the use of the RZWQM2 model to predict tile drainage flow and its impact on drainage water quality once calibrated to suit local conditions.

2.2.3.2 Manure and Fertilizer Application

Kumar et al., (1998b) found the RZWQM model to have satisfactorily simulated the effect of swine manure applications on [NO_3^--N] in subsurface drainage water from continuous corn fields (IA, USA) receiving a manure application. In another study, Ma et al., (1998a) used RZWQM to simulate the fate and transport of N attending the application of poultry manure in an agricultural field located at Arkansas, USA. The model adequately predicted the responses of soil profile [NO_3^--N]to poultry manure applications and corroborated RZWQM's ability to simulate manure dynamics. The RZWQM evaluation of soil [NO_3^--N] response to cattle manure application on a corn field located at Colorado, USA also demonstrated the model's ability to adequately predict soil [NO_3^--N] and soil water content ($r^2 > 0.83$, Ma et al., 1998b). Similarly, Malone et al., (2007) applied the RZWQM model to quantify the long-term effects of different types of N inputs (e.g., chemical fertilizer, swine manure), along with the timing and rates of their application on crop production and water quality in subsurface drainage water. They suggested that after proper calibration and thorough testing, the RZWQM model can be used to quantify the relative effects of corn production and [NO_3^--N]in tile drainage water under several alternative management practices. Qi et al., (2012) conducted a long-term simulation using RZWQM2 to investigate the impact of different N fertilizer application rates on N loss in a subsurface drainage system in north-central Iowa, USA and suggested an N application rate to meet the requirement of Iowa water quality standards. Again, the RZWQM2 model was shown to perform satisfactorily in simulating the response of [NO_3^--N] in subsurface drainage to nine different N fertilizer rates. This study strengthened the argument for using RZWQM2 to predict [NO_3^--N] in subsurface drainage at various N application rates, provided the model were calibrated for local conditions. Recently, Bhar and Kumar (2019) successfully applied RZWQM2 to predict real-time fertilization and irrigation decision-making for optimum crop production without environmental over-exploitation. From all these studies one can infer that RZWQM can simulate the impact of manure and fertilizer applications on water quality in different weather and soil conditions.

2.2.3.3 Pesticide Application

A limited number of studies have been found in the literature regarding the performance of RZWQM2 in estimating pesticide transport under different weather and soil conditions. Kumar et al., (1998a) calibrated and validated the RZWQM model using observed daily drainage and atrazine concentration data from Nashua, IA, obtained under two different tillage systems. Drawing on data from the same location in Iowa, Malone et al., (2014) later evaluated the model's ability to simulate pesticide transport. Both studies revealed that simulated drainage flow, and pesticide loss to tile drains closely followed the measured values and that simulated pesticide concentrations were comparable with observed values. In between, Ma et al., (2004) used RZWQM to investigate the loss of atrazine, alachlor and fenamiphos through surface runoff from conventional-tillage corn mesoplots located in Tifton, GA, US. The model effectively estimated runoff water volumes, resulting a predicted/observed ratio of 1.2 (±0.5) for all events. Predicted pesticide concentrations and loads were generally within a factor of 2, but atrazine losses from these events were underestimated. The ratios of predicted to measured pesticide concentrations in all runoff events varied between 0.2 and 147, with an average of 7. The normalized RMSE for pesticide runoff concentration and load predictions varied between 42 and 122%, with an average of 84%. The study concluded that the RZWQM's runoff mixing model delivers a reasonable estimate of pesticides loads and concentration in runoff water, provided that the pesticides are in dissolved/adsorbed forms and not in residual granules or ionized forms. Shrestha and Dutta (2015) tested and subsequently compared the performance of the RZWQM and PESTFADE (PESTicide Fate And Dynamics in the Environment) models in predicting soil water content, metribuzin fate, and transport in a sprinkler-irrigated soybean field located at the experimental farm of the Asian Institute of Technology (AIT) in the Pathumthani Province, Thailand. RZWQM performed better in simulating the soil water content, whereas the PESTFADE performed better in simulating the level of metribuzin residues in the soil. The RZWQM model slightly overpredicted the metribuzin residue at 0-0.10 m soil depth one day after pesticide application, whereas its prediction of metribuzin residues at 0.10-0.20 and 0.30-0.40 m soil depths concurred with measured values. The study concluded that with proper calibration the RZWQM model can be effectively applied to predict the movement of water and metribuzin residues in the soils of tropical zones. All these studies imply that the pesticide sub-models in RZWQM represent a robust predictor of pesticide entrainment and can be applied to various agro-climatic scenarios.

2.2.3.4 Water Table Management

Water table management practices, such as controlled drainage with or without subsurface irrigation systems, have been reported to be an effective way to improve agricultural water quality (Madramootoo et al., 2001; Drury et al., 2014). RZWQM has been successfully applied as a tool to develop suitable water table management practices under different weather and soil conditions. When Ma et al., (2007a) applied RZWQM to evaluate the long-term effects of crop rotation, tillage, and controlled drainage on crop yield and NO_3^--N loss through tile drain flow at Nashua, IA,USA, the model's simulation suggested that implementation of controlled drainage would result in a 30% reduction in drain flow and a 29% decrease in N losses in drain flow compared to free drainage. The RZWQM simulations closely agreed with observations, and the study concluded that RZWQM was a promising tool for quantifying the relative effects of controlled drainage on N loss in drainage flow. Based on a long-term RZWQM simulation (1996–2008), Fang et al., (2012) studied the effects of controlled drainage on N loss to subsurface drainage and reported that RZWQM was well capable of simulating the effect of controlled drainage on drainage water quality and would reduce N losses by 39% after switching from free drainage. Thorp et al., (2007, 2008) applied the RZWQM to understand how different water table management strategies might affect the water balance and N cycling across 48 different locations in the US Midwest and serve as a reference for water table management's impact on reducing N losses through drainage across different locations in the United States. The evaluation of RZWQM2 by Lu (2015) in simulating surface runoff from a subsurface drained field in Ontario, Canada reported that the model's simulation of surface runoff in a field under free drainage conditions was satisfactory but for the controlled drainage with sub-irrigation field the simulation was poor. In a study, Jiang et al., (2018) applied RZWQM2 to simulate the hydrologic cycle and crop production in a subsurface-drained and sub-irrigated field in Southern Quebec, Canada. The model showed a satisfactory simulation of soil water content, sap flow, growth stage, leaf area index, and crop yield. Tile flow simulations for both free drainage and controlled drainage with sub-irrigation were reasonably accurate during the growing season but, significantly overestimated flow during the non-growing season; accordingly, they applied a Kalman filter technique to improve the model's performance during the non-growing season. Overall, the study suggested that the RZWQM2 model implementing the Kalman filter technique can be used for water table management. Most recently, Jiang et al., (2020), implemented the hybrid RZWQM2-SHAW model to evaluate the model performance in predicting surface runoff, subsurface tile drainage, and crop yield under regular drainage and controlled drainage with sub-irrigation using data collected in a tile-drained field in Harrow, Ontario. The study demonstrated, RZWQM2-SHAW's satisfactory performance in simulating the subsurface drainage and runoff under both regular drainage and controlled drainage with sub-irrigation.

2.2.3.5 Tillage and Cropping System Management

The RZWQM2 model has been widely employed to investigate the impacts of tillage and cropping system management — including crop rotations, winter cover crops and crop residue removal — on water quality and crop production. Ma et al., (2007b) used the RZWQM model to evaluate year to year crop yield, water, and N balances in a study drawing on 26 years of data from a study near Nashua, IA. Although, average yields were fairly well simulated by the model, but yearly crop yields were less well simulated (r^2 = 0.52 for corn and r^2 = 0.37 for soybean). The model appropriately simulated year to year variations in tile flow (r^2 = 0.74) and N loading in tile flow (r^2 = 0.71). Simulated corn and soybean yields had high RMSE values (1386 and 674 kg ha^{-1}, respectively)1 with coefficient of variations (CV) of 0.19 and 0.25, respectively, while the RMSE for simulated soil water storage, water table, annual tile flow, annual N loading and residual soil N were 3.0 cm, 22.1 cm, and 5.6 cm, 16.8 kg N ha^{-1} and 47.0 kg N ha^{-1} respectively. The study concluded that further improvements in model algorithms were needed to better simulate plant N uptake and yield, but that overall, the use of RZWQM for the simulation of annual tile flow and annual N loading in tile flow was acceptable. In another study using RZWQM at the same location Ma et al., (2007a) evaluated the long-term management impacts of tillage and crop rotation on hydrology and crop yield, showing an adequate simulation of higher corn yield under a corn–soybean rotation than under continuous corn. The RZWQM model satisfactorily captured the observed increase in [NO_3^--N] in drain flow with increasing tillage intensity and showed 14% less drainage under the corn–soybean rotation than under continuous corn. The study concluded that RZWQM is a promising tool for quantifying the relative effects of tillage and crop rotation on N loss in drainage flow. Ahmed et al., (2007b) employed RZWQM to simulate the long-term effects of current N management practices for corn production in Southern Ontario, Canada and evaluated different cropping systems for their potentially better N management. The model satisfactorily simulated the amount of subsurface tile drainage, residual soil NO_3^--N, NO_3^--N in subsurface drainage water, and crop yield. Moreover, the simulation found that changing the crop rotation from corn-soybean to corn-soybean-soybean would result in a greater reduction in N losses through drainage on a silt loam soil than on a sandy loam soil. Using the RZWQM2 model (coupled with CERES-Wheat), Qi et al., (2013) conducted a study at Sydney, Montana to quantify the effects of crop management practices and tillage on soil water and spring wheat production in a continuous spring wheat system under dryland conditions. They further extended the RZWQM2 model simulation results to propose alternate cropping systems and management practices under long term weather conditions. The RZWQM2 model simulated soil water and crop yield to an acceptable level under various tillage methods, planting dates, and seeding rates, showed no impacts of tillage, but found late planting to considerably reduced grain yield and biomass. The model's simulation under long-term climate variability revealed a large water deficit (323 mm) for spring wheat and subsequently proposed a mitigation strategy consisting of fallowing the cropland every other year, which would conserve 42 mm of water for the following wheat growing season, resulting in a yield increase of 249 kg ha^{-1} (13.7%). Other long-term simulations identified that to achieve optimum economic returns optimal spring wheat planting dates should be between 1 March and 10 April, at seeding rates of 3.71 and 3.95×10^6 seeds ha^{-1} for conventional and ecological management treatments, respectively. Ding et al., (2020) employed RZWQM2, to simulate the effects of conventional tillage *vs.* four different conservation tillage practices (no-till, subsoiling tillage, no-till with straw, and subsoiling tillage with straw) on soil water, nitrogen dynamics, and yield of winter wheat in Henan province, China. They found an acceptable agreement index (*d*) and RMSE between simulated and measured soil water content, soil [NO_3^--N], and grain yield. The study demonstrated a reasonable use of the RZWQM2 model to simulate the impact of tillage on crop production, while it suggested replacing conventional tillage with no-till in Henan Province of China to reduce water loss and N leaching. Using RZWQM2, Qi et al., (2011) investigated the long-term impact of winter rye cover on water cycling and N dynamics under a soybean-corn rotation system at an experimental site located in Iowa, USA. Prior to the long-term simulation, the model was calibrated and validated against daily drainage flow under four different treatments. The model's simulation of drainage as well as NO_3^--N loss through tile drainage were deemed to be satisfactory. The results of long-term simulation indicated that a winter rye cover crop reduced annual subsurface drainage and NO_3^--N loss by 11% (29 mm) and 22% (11.8 kg N ha^{-1}), respectively, and increased annual ET by 5% (29 mm). Instituting the use of RZWQM to simulate the impact of cover crops on water quality in the Mississippi River Basin, and simulating corn–soybean rotations and continuous corn plantings in Ohio, Indiana, Illinois, Iowa, and Minnesota, Kladivko et al., (2014) showed 20% less N loss to the Mississippi River under a winter rye cover crop. In another recent study, Gillette et al., (2018) used the RZWQM model to evaluate NO_3^--N losses to drain flow and N_2O emissions in a corn-soybean system with a winter rye cover crop situated in central Iowa, USA and found that average measured and RZWQM simulated drain flow and [NO_3^--N] with a winter rye cover crop to be 60% and 54% less than without cover crop. Average annual April through October cumulative observed and simulated N_2O emissions were 6.7 and 6.0 kg N_2O-N ha^{-1} for no cover crop, and 6.2 and 7.2 kg N ha^{-1} for with a cover crop. The study concluded that RZWQM was a promising tool for estimating the impact of a winter rye cover crop on drainage water quality (NO_3^--NNO_3^--N) and N_2O emissions from subsurface drained agricultural fields under a corn-soybean rotation.

2.3 KNOWLEDGE GAP AND NEED OF RESEARCH

We still, today, face significant environmental problems with the nonpoint source P pollution of surface water bodies. The P pollution of surface water bodies is leading to eutrophication or algal bloom. Researchers have identified that agriculture fields are one of the major sources of P that eventually contributes to the surface water bodies. It is also identified that, among the agricultural fields, those are having artificial subsurface tile drainage system, contributes most towards this P loss. As of present, we still lack the extensive body of knowledge on the science behind the agricultural P dynamics and the fate and transport of P from an agricultural field. It is primarily because of the several limitations in the existing agricultural process control models (Radcliff et al., 2015) that can be effectively employed to simulate agricultural P dynamics and P loss from an agricultural field particularly through tile drainage system. The existing P models are mostly limited to surface runoff bound P losses simulation and does not have the capabilities to simulate P dynamics arising out of fertilizer / manure application. Many of the existing models also lacks the ability to simulate PP losses, which constitute majority of P loading originating from the agricultural fields. Researchers (Kleinman et al., 2015) have suggested that there is an urgent need to develop agricultural process control models particularly for the tiled drained agricultural filed that can be effectively used my the agricultural managers and planners to understand science behind the fate and transport of P from the agricultural field to the surface water bodies. This research is undertaken to overcome these limitations of the existing agricultural P simulation models (Radcliff et al., 2015), while developing an all-in-one P simulation model (RZWQM2-P) for the tile drained agricultural field as recommended by the earlier researchers (Kleinman et al., 2015). The developed RZWQM2-P model can serve as a valuable tool for agricultural planner and environmental scientists to evaluate different agricultural management practices and judicially identify best management practices to reduce P loading from agricultural field to the surface water bodies.

CONNECTING TEXT TO CHAPTER 3

Chapter 2 reviewed of some available P models and highlighted their limitations. The chapter 2 also discussed the RZWQM2 model's effective applications to simulate the impact of wide range of agricultural management practices on hydrology, crop growth and water quality and how its various features can be effectively used to develop a new P model to overcome the limitations of the exiting P models. The Chapter 3 presents the development and the first attempt of evaluating the newly developed P model (RZWQM2-P) (Root Zone Water Quality Model-Phosphorus) using a measured dataset including subsurface tile drainage, surface runoff, DRP and PP loss through tile drainage and surface runoff, soil water content, soil temperature from a corn soybean rotated, inorganic fertilizer applied artificially drained experimental field.

The following manuscript based on the content of the Chapter 3 has been published in the journal of Environmental Modelling and Software and it was co-authored by Zhiming Qi[1], Tie-Quan Zhang[2], Chin S. Tan[2], Liwang Ma[3] and Allan A. Andales[4].

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1. Department of Bioresource Engineering, McGill University, Sainte-Anne-de-Bellevue, Quebec, H9X 3V9, Canada

2. Harrow Research and Development Center, Agriculture and Agri-Food Canada, Harrow, Ontario, N0R 1G0, Canada

3. USDA-ARS Rangeland Resources and Systems Research Unit, Fort Collins, Colorado, 80526, USA.

4. Department of Soil and Crop Sciences, Colorado State University, Fort Collins, Colorado, 80523, USA.

CHAPTER 3

DEVELOPMENT AND EVALUATION OF A PHOSPHORUS (P) MODULE IN RZWQM2 FOR PHOSPHORUS MANAGEMENT IN AGRICULTURAL FIELDS

Debasis Sadhukhan[1], Zhiming Qi[1], Tie-Quan Zhang[2], Chin S. Tan[2], Liwang Ma[3] and Allan A. Andales[4]

1. Department of Bioresource Engineering, McGill University, Sainte-Anne-de-Bellevue, Quebec, H9X 3V9, Canada
2. Harrow Research and Development Center, Agriculture and Agri-Food Canada, Harrow, Ontario, N0R 1G0, Canada
3. USDA-ARS Rangeland Resources and Systems Research Unit, Fort Collins, Colorado, 80526, USA.
4. Department of Soil and Crop Sciences, Colorado State University, Fort Collins, Colorado, 80523, USA.

ABSTRACT

A few management tools can simultaneously describe dissolved and particulate P losses from tile-drained agricultural fields. In this study a phosphorus (P) management tool was developed based on most recent scientific findings to simulate dissolved and particulate P loses from tiled drained agricultural fields, and it was subsequently incorporated into the Root Zone Water Quality Model 2 (RZWQM2) to take advantage of its featured hydrologic and agricultural management subroutines. The RZWQM2-P model was evaluated against data collected in a tile-drained corn-soybean rotated field fertilized with inorganic P at South Woodslee, Ontario. The results indicate that overall, the model satisfactorily simulated dissolved reactive P (DRP) and particulate P (PP) losses through surface runoff and tile drainage with Nash-Sutcliffe model efficiency coefficient > 0.65, percent bias within 25% and index of agreement > 0.75. RZWQM2-P is a promising tool for P management, particularly for subsurface-drained fields. Further testing is needed to assess its performance under different fertilization (manure), soil, climate, and cropping conditions.

3.1 INTRODUCTION

Agriculture phosphorus (P) demand accounts for 80% to 90% of global phosphorus consumption. The supply of P is heavily dependent on mined rock phosphate, a non-renewable resource becoming increasingly scarce and expensive day by day. In plants, phosphorus plays a role in cellular energy transfer, respiration, and photosynthesis; and is a structural component of the nucleic acids of genes and chromosomes, as well as many coenzymes, phosphoproteins and phospholipids (Grant et al., 2001). While proper crop growth and the maintenance of high yields are critical to agricultural production, crop P use efficiency in the year of application is rather low (15-30%; Syers et al., 2008). The build-up of legacy P in soils under long-term application has increasingly caused P losses from soil to surface waters. Such P losses from agricultural fields via water and sediment have become a serious environmental concern, degrading the quality of water in fresh water bodies (*e.g.*, lakes and rivers), as well as brackish sea waters (*e.g.* sea coast rivers outlets), by causing a rapid increase in algal populations leading to eutrophication (Guildford and Hecky, 2000). Such algae infested water is resulting in adverse ecological conditions for aquatic flora and fauna. It is now an established fact that excessive P loading of freshwater bodies and coastal sea areas can be confidently attributed to an over application of fertilizer in upstream agricultural fields. It is estimated that 80% of the P pollution reaching Lake Champlain's Missisquoi Bay originated in upstream agricultural lands (Hegman et al., 1999). In Quebec alone, some 156 lakes were already deemed polluted by P (MSSS, 2007).

As removal of excess P from water by chemical (Surampalli et al., 1995) or biological (Oehmen et al., 2007) means is complex, expensive and time consuming, remediation of eutrophication in rivers and lakes is difficult. One practical option to mitigate this problem is to arrest P loss right at the source by adopting proper agricultural management practices. To control P loss from an agricultural field one must understand the P dynamics of an agricultural field. Kleinman et al., (2015) indicated that computer modelling drawing on measured P data was a currently priority in achieving this goal. Of available agricultural P management models, ICECREAM (Tattari et al., 2001) seems to be the best at simulating P losses through tile drains (Radcliffe et al., 2015). However, in the absence of a water table-based tile drainage component, ICECREAM uses matrix and macropore flow flux at a certain soil depth to mimic tile drainage (Qi and Qi, 2016; Radcliffe et al., 2015). ICECREAM adopts simple storage routing concepts to simulate matrix flow within the soil profile. This can be improved by adopting the soil-matric-potential-based Richards equation (Richards, 1931) to simulate matrix flow and Hooghoudt's equation (Bouwer and Schilfgaarde, 1963) to simulate tile drainage. With no separate P pool to simulate manure and fertilizer P dynamics, ICECREAM assumes that manure or fertilizer P are mixed with the soil upon application.

Modelling P in an agricultural field involves modelling of hydrological processes on and below the ground surface and the effects of agricultural management practices. A P model needs to simulate both surface hydrological processes (*e.g.*, soil evaporation, plant transpiration, runoff, and soil erosion), and subsurface hydrological processes (*e.g.*, infiltration, matrix flow, preferential flow or macropore flow, flow to tile drainage, fluctuation of water tables, root water and nutrient uptake, and soil moisture redistribution). Agricultural management practices such as surface irrigation and sub-irrigation, drainage, fertilization, tillage and residue management, and crop rotation influence the fate and transport of P. The success of a P model greatly depends on how effectively and efficiently the model captures these hydrological processes and how these processes are parameterized within the model. RZWQM2 (Ahuja et al., 2000), a widely tested field-scale process-based model, is an ideal option as a base of a P model, because it is equipped with subroutines to simulate all the hydrological processes and agricultural management practices mentioned above. It has been extensively evaluated at locations across the United States (Fang et al., 2014a,b; Gillette et al., 2018; Hanson et al., 1999; Ma et al., 2007 a,b, 2004; Malone et al., 2014; Qi et al., 2011, 2012, 2013; Thorp et al., 2007; Wang et al., 2015) and in Canada (Ahmed et al., 2007a, b; Al-Abed et al., 1997; Madani et al., 2002; Jiang et al., 2018). Nonetheless, current P models lack the capacity to adequately simulate P losses, particularly those occurring through tile drainage (Radcliffe et al., 2015). In this study an attempt was made to develop a model based on most recent scientific finding regarding the fate and transport of P from an agricultural field available in the literature, and to test this new P management tool against measured hydrologic and P data in a tile-drained cropland.

3.2 MATERIALS AND METHODS

3.2.1 P Model

The P model (Figure 3.1) is designed with five different soil P pools: three inorganic, namely labile P (LabP) active inorganic P (ActIP) and stable inorganic P (StabIP) and two organic pools namely fresh organic P pool (FresOP) and stable organic P pool (StabOP) respectively following the nomenclature of Jones et al., (1984). Besides these soil P pools, as an advanced feature the model also has four surface manure P pools and two surface fertilizer P pools to simulate P dynamics arising from the application of fertilizer and manure (Vadas, 2014). The manure P pools are inorganic water extractable P (ManWIP), inorganic stable P (ManSIP), organic water extractable P (ManWOP), and organic stable P (ManSOP). The fertilizer P pools were available fertilizer P (AvFertP) and residual fertilizer P (ResFertP) Among these P pools, the LabP pool is considered to be in dissolved form and the most dynamic P pool. In addition, it is the only P pool from which plants can uptake P. Plant root density is the highest near the soil surface so plant P uptake in the upper portion of the soil profile is more than that in deeper layers. This depth distribution of plant P uptake is controlled by plant P uptake distribution parameter. The governing equations of plant P uptake were adopted from Neitsch et al., (2011). There is constant absorption and desorption happen among these three inorganic P pools to maintain an equilibrium. The LabP pool is in rapid equilibrium with the $ActIP$ pool, which is in slow equilibrium with the StabIP pool. The rapid adsorption and desorption of inorganic P in the soil between LabP and ActIP is simulated based on Jones et al., (1984), with advanced dynamic absorption and desorption as prescribed by Vadas et al., (2006). This modification enables the model to simulate P movement among these pools by using a dynamically changing rate factor rather than a constant rate factor. The slow adsorption and desorption of inorganic P in the soil between ActIP and StabIP is simulated based on Jones et al., (1984). After decomposition, P from plant residues and soil humus are added to the FresOP pool and the StabOP pool, respectively. Mineralization happens from FresOP pool and mineralized P is added to the LabP and the StabOP pools. A slow mineralization also follows in the StaOP pool and mineralized P is added to the LabP pool. Immobilization happens in the LabP pool and immobilized P is added to the FreOP pool. When fertilizer and/or manure is applied in the field the fertilizer and/or manure P is subsequently added to the fertilizer and manure pools based on application depth, type and properties of fertilizer and/or manure applied (Vadas, 2014). These independent fertilizer and manure P pools enable the model to simulate more precisely the P dynamics arising from the application of fertilizer and manure in an agricultural field. Then the leaching and decomposition takes place from these pools. Decomposed and leached P are added to the soil P pools. The ability of the P model to simulate DRP through tile flow is improved by adopting the recommendations of Francesconi et al., (2016) whereas the PP loss through tile drainage is simulated by considering colloidal particle transport through macropore flow (Jarvis et al., 1999; Larsson et al., 2007). In the model, the first soil layer is set to a 0.01 m depth as the model assumes that particle bound P originates from the first 0.01 m depth of the soil profile. All the P pools contribute to PP loss whereas the LabP pool, ManWOP and ManWIP pools and all the ferilizer P pools contribute to DRP loss. To simulate DRP and PP loss through tile drainage the linear groundwater reservoir-based approach, as suggested by Steenhuis et al., (1997), was used. In this approach DRP is generated through matrix flow and macropore flow, while PP is only generated through macropore flow and is first to contribute to a groundwater reservoir. Subsequently a daily mass balance is calculated, then DRP and PP is lost along with the tile drainage water from this groundwater reservoir. All the equations used in the model are provided in the Appendix A.

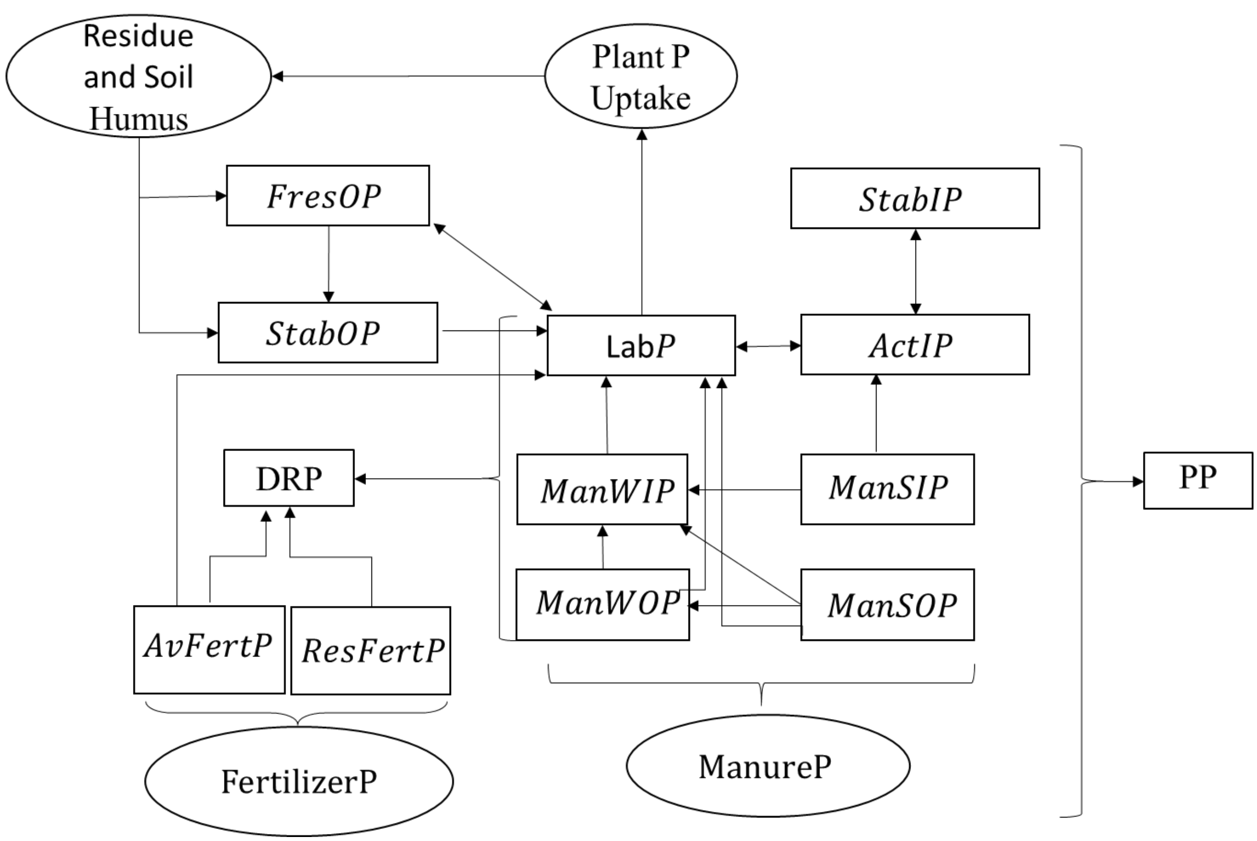

Figure 3.1: RZWQM2-P Model's P pools.

FresOP , fresh organic P; StabOP, stable organic P; StabIP, stable inorganic P; ActIP, active inorganic P; LabP, labile P pool; ManWIP, manure water extractable inorganic P; ManWIP, manure water extractable organic P; ManSIP, manure stable inorganic P; ManSOP, manure stable organic P; AvFertP available fertilizer P; ResFertP, residual fertilizer P; DRP,dissolved reactive P; PP, particulate P; FertilizerP, Applied P with fertilizer application; ManureP, Applied P with manure application.

3.2.2 RZWQM2 Overview

Developed by the USDA-ARS, the RZWQM2 model (Ahuja et al., 2000) is a field scale, one-dimensional model which integrates physical, biological, chemical and hydrological processes and simulates crop growth, hydrologic cycle, fate and transport of nutrients and pesticides under different agronomic management practices and climate patterns. Within the RZWQM2 model soil water retention is described using the Brooks-Corey equation (Brooks and Corey, 1964). The Green-Ampt approach (Green and Ampt, 1911) is used to compute the infiltration. The model employs the Richards equation (Richards, 1931) to simulate soil water redistribution following infiltration in the soil profile. Tile drainage flow is calculated by Hooghoudt's steady state equation (Bouwer and Schilfgaarde, 1963) and the macropore flow is governed by the Poiseuille's law. The Simultaneous Heat and Water (SHAW) model (Flerchinger, 1987,1989) is linked to RZWQM2 to simulate ice in soil, snow accumulation, snow melting, as well as soil freeze-thaw cycles. The crop growth can be simulated either by embedded DSSAT 4.0 crop models (Jones et al., 2003) or a generic crop production model (Hanson, 2000) whereas evapotranspiration is estimated using the double layer Shuttleworth-Wallace model (Shuttleworth and Wallace, 1985).

3.2.3 P model and RZWQM2 Integration

The P model described above was first developed then incorporated into the RZWQM2 model. While the P model simulates P dynamics, the RZWQM2 governs the physical, biological, chemical and hydrological processes that influence the P simulation. The developed P model combined with RZWQM2 performs as a single tool, the P model being dependent on RZWQM2 for the simulation of crop growth, runoff, drainage, soil moisture and its flux, soil temperature, sediment yield, macropore flow, residue and soil humus decomposition and agriculture management practices. All these components are simulated by RZWQM2 within its original functionalities and then the P model uses model outputs to simulate P dynamics and P loss through surface runoff and tile drainage from an agricultural field. The P model's working algorithms along with its dependencies on RZWQM2 are presented in Figure 3.2.

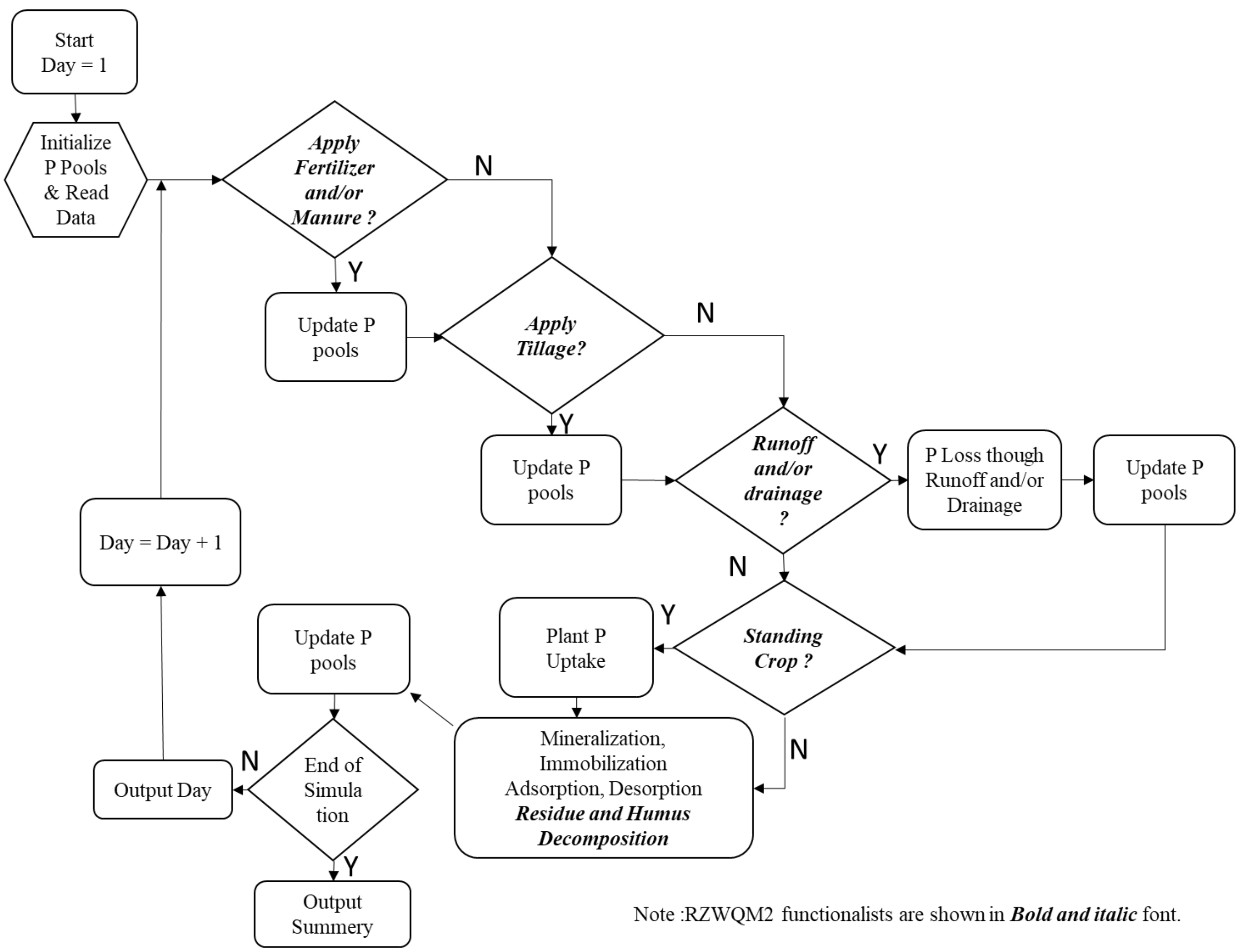

Figure 3.2: RZWQM2-P model's working algorithms and its dependencies on RZWQM2

3.2.4 Field Experiment

To evaluate the P model, observed runoff and drainage water flow, as well as DRP and PP mass in both runoff and tile drainage water were collected from an Agriculture Agri-Food Canada (AAFC) experimental site, the Hon. Eugene F. Whelan Research Farm, near South Woodslee, ON (42.21N, 82.74W) from June 2008 to December 2012. The site was comprised of 16 plots (67.1 m × 15.2 m) receiving different fertilizer types and drainage system treatments. Among these, plot numbers 5 and 9, selected for the present study, received inorganic NPK fertilizer applications and were subject to standard tile drainage (depth: 0.85 m, spacing: 3.8 m) (Zhang et al., 2013). The crop was rotated between maize (*Zea mays* L.) and soybean [*Glycine max* (L.) *Merr.*] in alternating years. In 2008, 2010 and 2012 maize was planted at a density of 79,800 seeds ha^{-1}, while in 2009 and 2011 soybean was planted at a at a density of 486,700 seeds ha^{-1}. The inorganic fertilizers (114.5 kg P_2O_5 ha^{-1} (roughly 50 kg P ha^{-1}), 200 kg N ha^{-1} from NH_4NO_3, and 100 kg K ha^{-1} from KCl) were surface-applied before planting in the maize planting years. Chisel plow tillage was done each year after harvest or in the following year before planting. The dates of cropping and other crop management practices are presented in Table 3.1. The P content in corn and soybean grain were measured after harvest (between 20 October and 13 December) each year. Grain samples were dried at 55°C, ground and passed through a 1-mm sieve and digested using a H_2SO_4-H_2O_2 procedure. Phosphorus concentrations in all of the filtrates and digests were determined using a QuikChem Flow Injection Auto-Analyzer (Lachat Instruments), employing the ammonium molybdate ascorbic acid reduction method (Murphy and Riley, 1962).

Table 3.1: Crop and management practices at the Site

Year	Date	Management practices
2008	08-Jun	Inorganic fertilizer
	18-Jun	Maize planting
	5-Nov	Maize harvest
2009	5-Mar	Chisel plow
	22-May	Soybean planting
	20-Oct	Soybean harvest
	1-Nov	Chisel plow
2010	17-Jun	Inorganic fertilizer
	26-Jun	Maize planting
	8-Nov	Maize harvest
	1-Dec	Chisel plow
2011	15-Jun	Soybean planting
	13-Dec	Soybean harvest
	20-Dec	Chisel plow
2012	20-May	Chisel plow
	22-May	Inorganic fertilizer
	25-May	Maize planting
	05-Nov	Maize harvest
	20-Nov	Chisel plow

The soil type was clay loam and the measured soil properties for plots 5 & 9 were averaged (Table 3.2) and used as the soil input data for the model. The soil profile was delineated into six layers. The soil properties such as soil texture, field capacity (θ_{fc}), permanent wilting point (θ_{wp}), and saturated hydraulic conductivity (k_{sat}) were measured before the start of the experiment. Soil bulk density (ρ) and porosity (φ) were measured in 2010 where as k_{sat} was measured in the year 2008. Prior to the onset of the experiment in 2008, soil P was measured using the Olsen P method (Olsen et al., 1954). Volumetric soil moistures (θ) for the soil layer ranging in depth between 0-0.08 m were measured twice a week using a portable probe, while soil temperature (T_{soil}) at depth of 0.05 m was measured hourly from June to October for the years 2010, 2011, and 2012, using sensors. Hourly T_{soil} were averaged to obtain daily mean T_{soil}.

Table 3.2: Model input data for soil physical and chemical properties, average of Plots 5 & 9

Soil Layer depth (m)	ρ ($Mg\ m^{-3}$)	Clay (%)	Sand (%)	OM (%)	θ_{fc} (m^3m^{-3})	φ ($m^3\ m^{-3}$)	θ_{wp} ($m^3\ m^{-3}$)	pH	LabP ($g\ kg^{-1}$)	FresOP ($g\ kg^{-1}$)	StabOP ($g\ kg^{-1}$)	TotalP ($g\ kg^{-1}$)
0.00-0.01	1.326	34.2	29.0	3.7	0.368	0.54	0.175	7.5	0.0230	0.100	0.2303	0.9045
0.01-0.10	1.326	34.2	29.0	3.7	0.368	0.54	0.175	7.5	0.0210	0.085	0.2174	0.9000
0.10-0.25	1.391	34.2	29.0	3.7	0.361	0.54	0.175	7.5	0.0210	0.085	0.2174	0.9000
0.25-0.45	1.391	40.7	25.7	2.0	0.351	0.50	0.175	7.5	0.0110	0.055	0.1148	0.6500
0.45-0.80	1.326	40.4	27.0	0.7	0.356	0.48	0.175	7.5	0.0055	0.028	0.0580	0.5000
0.80-1.20	1.326	39.3	24.6	0.5	0.356	0.48	0.174	7.5	0.0055	0.028	0.0580	0.4000

ρ, soil bulk density; Clay, soil clay content; Sand, Soil Sand Content; OM, Soil organic matter content; θ_{fc}, Volumetric soil moisture content at field capacity; φ, Soil Porosity; θ_{wp}, Volumetric soil moisture content at permanent wilting point; pH, soil pH; LabP, Soil labile P, FresOP, Soil fresh organic P, StabOP, soil stable organic P ; TotalP, Soil total P.

The required weather data (air temperature, precipitation, relative humidity, solar radiation and wind speed) to run the model were collected for the period of 1st Jan. 2008 to 31st Dec. 2012 from the automated meteorological weather station located at the Whelan farm, located less than 500 m from the experimental site. During the winter (1st Oct. – 30th April of 2009, 2010 and 2011), rain gauge inaccuracies for snowfall precipitation, led to data being obtained from Environment Canada's Harrow Weather Station (Station ID 6133362, 42.03^{0}N, 82.90 ^{0}W) located 16.6 km from the study field. In each experimental plot there was a catch basin similar to a sewage sink at their downstream end to collect the surface runoff. Surface runoff and tile drainage from the experimental plot were directed to a central instrumentation building via underground PVC pipes. In the instrumentation building, the flow rate was measured automatically using electronic flowmeters and recorded in a multi-channel data logger. Surface runoff and tile drainage water samples were collected automatically using autosamplers (CALPSO 2000S, Buhler Gmbh & Company). Surface and tile water samples were collected continuously (year-round), proportionally to flow volume, samples being taken for every 1000 L of flow during the growing season and for every 3000 L of flow during the non-growing seasons. After the collection the samples were analyzed in the laboratory for DRP and total dissolved P ($TotalDP$) using an acidified ammonium persulfate [$(NH4)_2S_2O_2$] oxidation procedure (USEPA, 1983). Unfiltered water samples were analyzed for total P (TotalP) using the sulfuric acid-hydrogen peroxide digestion method (USEPA, 1983). The PP was computed by the difference between TotalP and TotalDP.

3.2.5 Model Calibration and Validation

The RZWQM2 with this newly developed P model was run using the four and a half years (June 2008 – Dec 2012) of data collected from the experimental site. There were some limitations on flow event separation during the flow data collection, so to ensure the precision of P loss estimation, the collected data was aggregated into 19 different periods (Table 3.3) and out of these the first twelve periods (01 June 2008 to 21 Dec 2010, two and half years) were used for calibrating the model, while the last seven periods (22 Dec 2010 to 09 Dec 2012, two years) were used for validating the model. During the calibration process, parameters related to soil moisture, soil temperature, surface runoff and tile drainage were initially calibrated, as these processes control the P loss from an agricultural field. Then the parameters related to P loss through surface runoff and tile drainage were calibrated. The calibration was undertaken manually while changing the calibration parameters within the range as obtained from prior studies and available literature, by a trial and error method following the protocol given by Ma et al., (2011) and iterated several times until a good match with the observed data was obtained. Three model evaluation statistics: Nash-Sutcliffe efficiency (NSE), percent bias (PBIAS), and Index of agreement (IoA) (Moriasi et al., 2007, 2015) served to evaluate the performance of the model in simulating hydrology, soil moisture, soil temperature and P loss through surface runoff and tile drainage. Model performance was catergorised as very good, good, statisfatory and unsatifactory based on the criterion of those model evaluation statistics as recommended by Moriasi et al., (2007, 2015). The model is regarded to perform satisfactorily when NSE > 0.50 and good when NSE > 0.65. Model performance is deemed to be satisfactory when |PBIAS| is between 15% and 25% for water flow and is between 40% and 70% for P and it is deemed to be good when |PBIAS| is between 10% and 15% for water flow and is between 25% and 40% for P (Moriasi et al., 2007). Model performance is regarded as acceptable when IoA > 0.75 (Moriasi et al., 2015).

Table 3.3: Periods of water flow and P measurement data for calibration and validation

Period no.	Period	Period no.	Period
	Calibration		Validation
1	1/Jun/2008-16/Jun/2008	13	22/Dec/2010-23/Mar/2011
2	17/Jun/2008-17/Jul/2008	14	24/Mar/2011-22/Jun/2011
3	18/Jul/2008-22/Oct/2008	15	23/Jun/2011-7/Sep/2011
4	23/Oct/2008-11Feb/2009	16	8/Sep/2011-7/Sep/2011
5	12/Feb/2009-27/Mar/2009	17	10/Nov/2011-22/Dec/2011
6	28/Mar/2009-26/May/2009	18	23/Dec/2011-12/May/2012
7	27/May/2009-16/Jul/2009	19	13/May/2012-09/Dec/2012
8	17/Jul/2009-23/Oct/2009		
9	24/Oct/2009-20/Apr/2010		
10	21/Apr/2010-11/Jun/2010		
11	12/Jun/2010-5/Aug/2010		
12	6/Aug/2010-21/Dec/2010		

In RZWQM2 model soil moisture content is parametrized with air entry pressure (P_b) and pore size distribution index (λ). Initially the values P_b and λ were set to the default values of these parameters according to soil texture as given by Ma et al., (2011) then subsequently these values were adjusted to match the observed values. The value of λ was found to be more sensitive than that of P_b in soil water simulations: an increase in λ resulted in reduction in soil water content whereas an increase of P_b led to increase of soil water content. Once the soil moisture content was calibrated and a good fit with the observed value was found, then calibration of runoff and tile drainage followed. To calibrate runoff parameters such as saturated hydraulic conductivity (k_{sat}), surface crust hydraulic conductivity (k_{crust}) and albedo were adjusted. In RZWQM2 runoff is simulated when the rainfall rate exceeds the infiltration rate (Ma et al., 2012), so the top layer k_{sat} and k_{crust} values were adjusted to obtain a good fit with the observed runoff. Furthermore, the albedo was adjusted for simulation of evapotranspiration, which in turn affected surface runoff. For tile drainage calibration, k_{sat}, P_b and lateral hydraulic conductivity (k_{lat}) were adjusted. Increasing k_{sat} resulted in an increase in tile drainage, whereas increasing P_b resulted in decrease in tile drainage. Moreover, k_{lat} had very prominent influence in tile drainage simulation and it was adjusted to $2\times k_{\mathrm{sat}}$. In addition, P_b was slightly adjusted to better match tile drainage without hampering the previous calibration for soil moisture.

The loss of DRP through surface runoff was calibrated by adjusting the soil P extraction coefficient while calibration of DRP loss through tile drainage depended on macroporosity, P_b and λ of the deeper soil layers. In the model, macropore flow is initiated when the top soil layer becomes saturated and DRP carried away through macropore flow depends on the volume of macropore flow. Therefore, to control the DRP loading to the groundwater reservoir the macroporosity value was adjusted. Finally, the P_b and λ of the deeper soil layers were slightly adjusted to control the DRP loading to groundwater reservoir by matrix flow without altering the earlier results for tile drainage and soil moisture simulations. The PP loss through surface runoff was calibrated by adjusting USLE soil loss coefficients (soil erodibility factor, cover and management factor, support practice factor) and Manning's n. These parameters control the sediment yield thereby controlling the PP loss through surface runoff. Increasing soil erodibility increased the sediment yield, while increasing the Manning's n reduced it. Accordingly, to obtain a good match of PP loss through surface runoff these two parameters were carefully adjusted along with the cover and management factor and support practice factor. The PP loss through tile drainage is controlled by parameters like soil replenishment rate coefficient, soil detachability coefficient, and soil filtration coefficient. These parameters govern the colloidal particle loss to sub-surface flow hence limit the PP loss through tile drainage. The high soil filtration coefficient leads to less colloidal particle loss whereas the increase of soil detachability coefficient and soil replenishment rate coefficient leads to more colloidal particle loss. So, these parameters were carefully balanced over the calibration period to get a reasonable simulation with respect to PP loss through tile drainage. Finally, to adjust the plant P uptake from the LabP pool, the P uptake distribution parameter for each crop was adjusted. Calibrated soil hydraulic parameters and their values are presented in Table 3.4 and all other calibrated parameters are presented in Table 3.5.

Table 3.4: Calibrated soil hydraulic parameters

Soil Layer depth (m)	Soil hydraulic parameters			
	P_b (cm)	λ	k_{sat} (cm hr^{-1})	k_{lat} (cm hr^{-1})
0.00-0.01	-20.06	0.16	0.25	0.50
0.01-0.10	-29.03	0.15	0.35	0.70
0.10-0.25	-14.64	0.20	0.55	1.10
0.25-0.45	-12.16	0.19	0.55	1.10
0.45-0.80	-25.10	0.15	0.17	0.34
0.80-1.20	-35.16	0.14	0.17	0.34

P_b, Air entry pressure; λ, Pore size index; k_{sat}, Saturated hydraulic conductivity; k_{lat}, Lateral Hydraulic Conductivity;

Table 3.5: Calibrated parameters and their values

Parameters	Calibrated Values	Default (Range)
Surface k_{crust} (mm h^{-1})	0.50	0.01 (0.01-20)
Albedo		
Dry soil	0.50	0.20 (0.01-0.9)
Wet Soil	0.65	0.30 (0.02-0.9)
Crop at Maturity	0.55	0.70 (0.01-0.9)
Fresh Residue	0.85	0.22 (0.01-0.9)
Macroporosity (m^3 m^{-3})	0.03	-
P extraction coefficient (-)	0.35	0.10-1.00
USLE Coefficients		
Soil erodibility (ton ac^{-1})	0.25	0.02(0.005-0.80)
Cover and management factor	0.85	0.50 (0.01-1.00)
Support practice factor	0.85	0.50 (0.01-1.00)
Manning's n	0.02	0.01 (0.01-0.40)
Soil filtration coefficient (m^{-1})	0.002	0.00 (0.00-1.00)
Soil detachability coefficient (gm J^{-1} mm^{-1})	0.90	0.40 (0.00-1.00)
Soil replenishment rate coefficient (gm m^{-2} day^{-1})	0.10	0.20 (0.00-1.00)
P uptake distribution parameter		
Corn	10.00	1.00-15.00
Soybean	10.00	1.00-15.00

3.3 RESULTS

3.3.1 Soil Moisture and Soil Temperature

The time series of simulated and observed soil temperature (T_{soil}) at 0.05 m depth and soil moisture (θ) between 0-0.08 m depths are presented in Figure 3.3. The simulation statistics are summarized in Table 3.6. Model simulation of θ and T_{soil} ware satisfactory with NSE of 0.64, PBIAS of 0.30% and IoA of 0.89 and with NSE of 0.59, PBIAS of 13.08 % and IoA of 0.89 respectively.

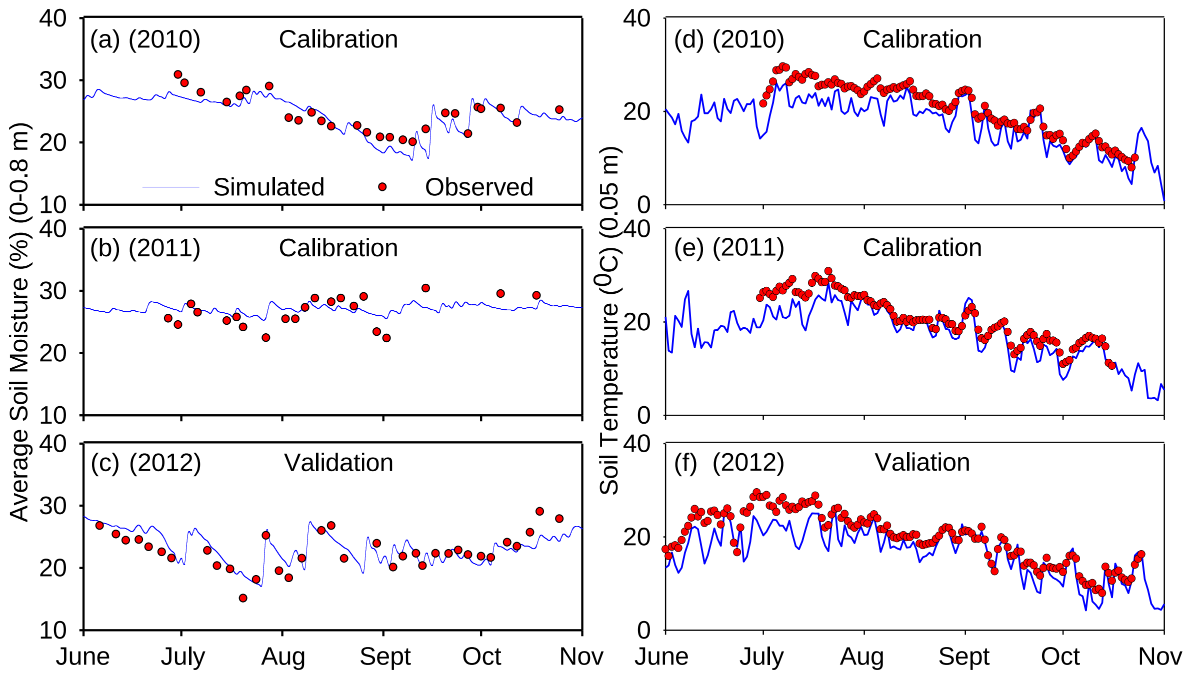

Figure 3.3: Comparison between simulated and observed (a, b, c) soil moisture (%) (0-0.08 m) and (d, e, f) soil temperature (^{0}C) (0.05 m)

Table 3.6: Statistics for model performance in Soil Moisture and Soil Temperature simulation

Statistics	Soil Moisture			Soil Temperature		
	Calibration	Validation	All Period	Calibration	Validation	All Period
PBIAS	1.63%	-1.67%	0.30%	12.67%	13.72%	13.08%
NSE	0.57	0.56	0.64	0.63	0.52	0.59
IoA	0.88	0.86	0.89	0.91	0.88	0.89

PBIAS, Percent bias, NSE, Nash-Sutcliffe model efficiency; IoA, Index of agreement.

3.3.2 Hydrology

Simulated *vs.* observed surface runoff and tile drainage are depicted in Figures 3.4a and 3.4b, respectively, and the accuracy statistics presented in Table 3.7. For the calibration period, simulation in surface runoff was very good and in tile flow was satisfactory based on the model evaluation criteria. During the calibration period, surface runoff was estimated with PBAIS of -12.47% and with NSE of 0.85 while drainage was estimated with PBAIS of 12.46% and the NSE of 0.60. The simulated average annual runoff and tile drainage were 129.57 mm and 375.43 mm (Table 3.8), respectively. These values were very close to the observed annual mean values. Overall, the model's performance was very good in simulating runoff (NSE>0.75, PBIAS within ± 10% and IoA > 0.75) and good in simulating tile drainage (NSE>0.65, PBIAS within ± 10% and IoA > 0.75). The simulated *vs.* observed water balance components are summarized in Table 3.8. During the four and a half years of simulation, simulated average annual ET (449.73 mm) was 47.45% of the observed annual precipitation (947.71 mm). This was similar to annual ET that was 45% of measured precipitation in the same region (Tan et al., 2002b). Between the simulated average annual surface runoff and tile drainage, most (74.34 %) of the water moved out of the field through the tile drainage system.

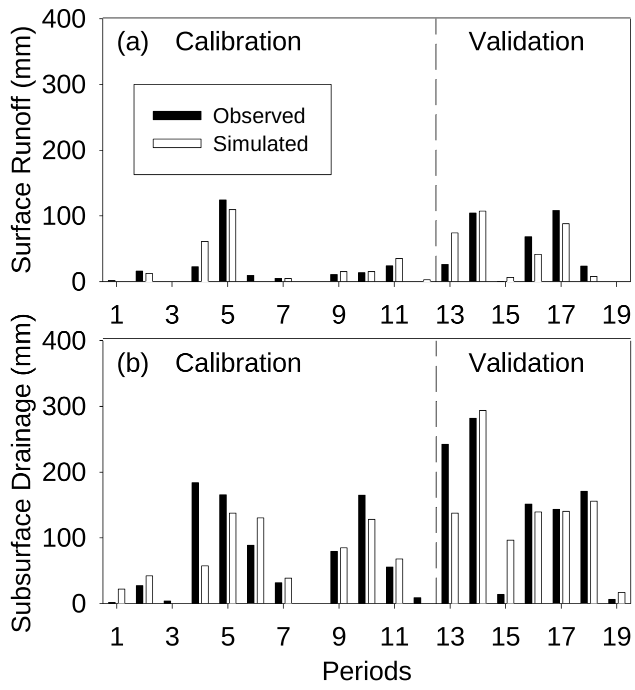

Figure 3.4: Comparison between simulated and observed (a) surface runoff (b) subsurface drainage. Periods are the time periods as mentioned in Table 3.3.

Table 3.7: Statistics for model performance in simulation of water, dissolved reactive phosphorus (DRP), particulate phosphorus (PP) and sum of DRP & PP (SumP)

Statistics	Runoff			Drainage		
Water						
	Calibration	Validation	All periods	Calibration	Validation	All periods
PBIAS	-12.47%	1.71%	-4.08%	12.46%	2.95%	7.18%
NSE	0.85	0.71	0.81	0.60	0.72	0.73
IoA	0.96	0.92	0.95	0.86	0.91	0.92
Dissolved Reactive P (DRP)						
	DRP in Runoff			DRP in Drainage		
	Calibration	Validation	All periods	Calibration	Validation	All periods
PBIAS	10.63%	-2.80%	4.58%	-13.40%	6.17%	-1.19%
NSE	0.95	0.59	0.80	0.65	0.74	0.83
IoA	0.99	0.90	0.95	0.91	0.94	0.95
Particulate Phosphorus (PP)						
	PP in Runoff			PP in Drainage		
	Calibration	Validation	All periods	Calibration	Validation	All periods
PBIAS	13.79%	-10.24%	0.10%	-8.28%	5.55%	0.54%
NSE	0.76	0.72	0.76	0.58	0.69	0.73
IoA	0.93	0.91	0.93	0.86	0.86	0.90
Sum of DRP and PP (SumP)						
	SumP in Runoff			SumP in Drainage		
	Calibration	Validation	All periods	Calibration	Validation	All periods
PBIAS	12.87%	-8.34%	1.40%	-10.15%	5.76%	-0.07%
NSE	0.84	0.73	0.78	0.71	0.84	0.86
IoA	0.96	0.92	0.94	0.92	0.94	0.95
	SumP in Runoff+ Drainage					
	Calibration	Validation	All periods			
PBIAS	-1.38%	1.59%	0.41%			
NSE	0.86	0.82	0.86			
IoA	0.96	0.94	0.95			

PBIAS, Percent bias, NSE, Nash-Sutcliffe model efficiency; IoA, Index of agreement. DRP, Dissolved Reactive Phosphorus; PP, Particulate Phosphorus; SumP, Sum of DRP, PP;

Table 3.8: Water balance table for simulation period (mm)

Year	Rainfall	ET	Runoff		Drainage		ΔS	Lateral	Deep
	OB		SIM	OBS	SIM	OBS		Flow	Seepage
06/01/08-05/26/09	1034.90	441.51	183.56	174.68	389.72	470.53	-4.56	0.00	8.69
05/26/09-06/11/10	721.20	417.68	35.56	29.72	251.64	275.73	-11.31	0.00	3.43
06/11/10-06/22/11	1171.50	422.96	219.26	154.82	499.38	588.51	-9.14	0.00	12.26
06/22/11-05/15/12	994.70	335.28	144.14	200.89	532.06	479.19	7.61	0.00	6.33
05/15/12-12/09/12	342.40	406.35	0.55	0.12	16.64	6.26	56.80	0.00	0.78
Total	4264.70	2023.80	583.07	560.23	1689.45	1820.22	39.40	0.00	31.49
Average (mm y-1)	947.71	449.73	129.57	124.50	375.43	404.49	8.76	0.00	7.00

OBS, Observed; SIM, Simulated; ET, Evapotranspiration; ΔS, Soil water change

3.3.3 Dissolved Reactive Phosphorus (DRP) Loss

Simulated and observed DRP loss through runoff and drainage for the calibration and validation periods are presented in Figures 3.5a & 3.5b and the simulation statistics are summarized in Table 3.7. The simulation statistics show that the P model's simulation of DRP loss through surface runoff during the calibration period was in very good agreement with the observed data (NSE >0.75, PBIAS within ± 25% and IoA > 0.75) whereas for tile drainage it was good (NSE >0.65, PBIAS within ± 25% and IoA > 0.75). During the validation period, simulated DRP loss through runoff was satisfactory and simulated DRP loss through tile drainage was good (Table 3.7). Overall the P model could simulate the DRP loss through both surface runoff and tile drainage in very good agreement with the observed data (NSE >0.75, PBIAS within ± 25% and IoA > 0.75) and it was found that most of the DRP (75.93% of total simulated DRP loss) was lost through the tile drainage system during the simulation period (Table 3.9).

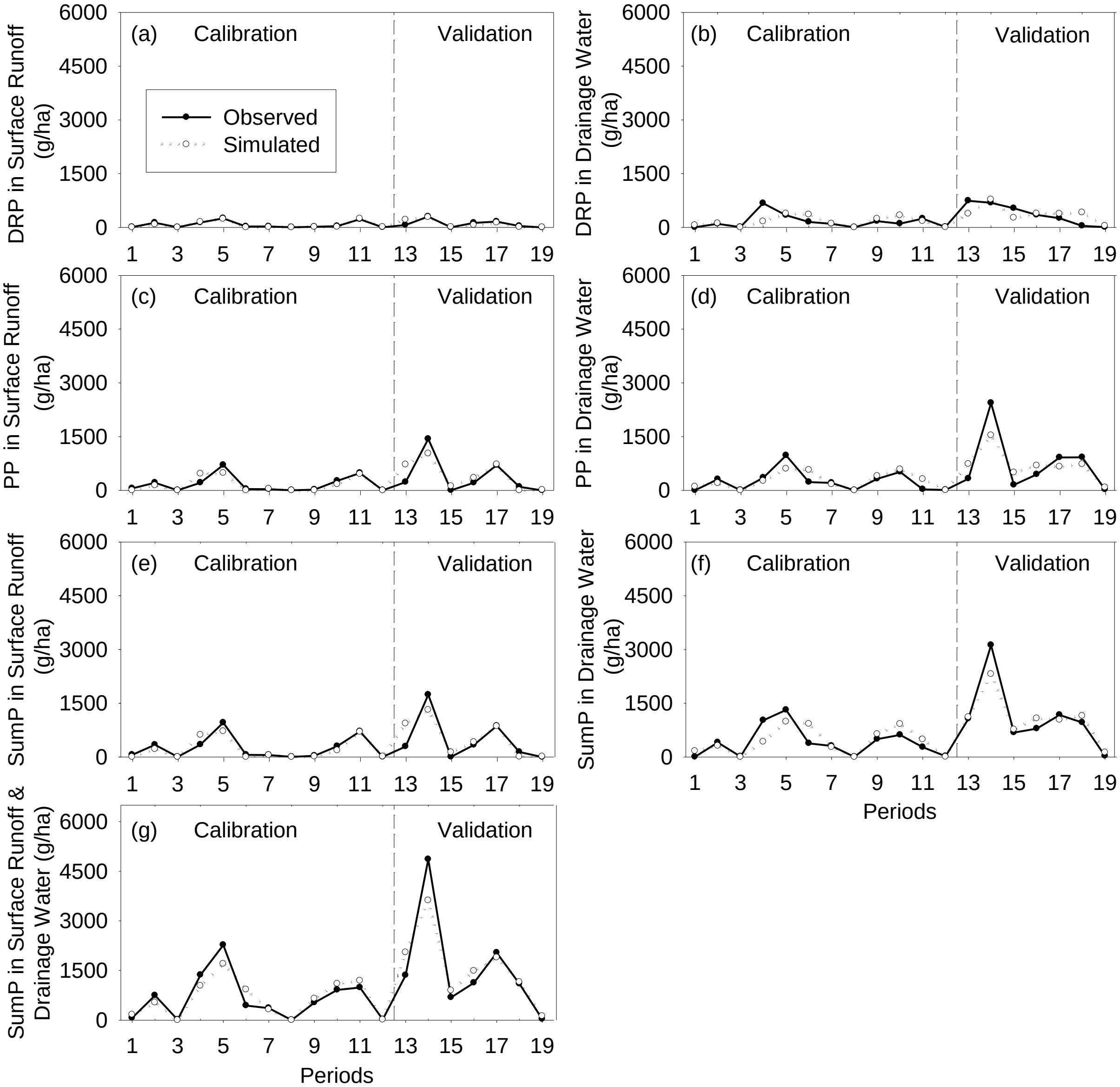

Figure 3.5: Comparison between simulated vs. observed mass of (a) DRP in surface runoff, (b) DRP in drainage water (c) PP in surface runoff, (d) PP in drainage water, (e) SumP in surface runoff, (f) SumP in drainage water, (g) SumP in surface runoff + drainage water. DRP, Dissolved Reactive Phosphorus; PP, Particulate Phosphorus; SumP, Sum of DRP, PP; Periods are the time periods as mentioned in Table 3.3.

Table 3.9: P balance table for the simulation period (all values in kg ha^{-1})

Year	Ferti-lizer	Residue & Humus P Release	GH		DRP				PP				ΔSP
					Runoff		Drainage		Runoff		Drainage		
			SIM	OBS	SIM	OBS	SIM	OBS	SIM	OBS	SIM	OBS	
06/01/08-05/26/09	50.00	21.50	19.56	15.30	0.47	0.54	1.07	1.27	1.08	1.22	1.73	1.87	34.46
05/26/09-06/11/10	0.00	33.11	20.12	18.26	0.03	0.07	0.68	0.37	0.21	0.32	1.15	1.04	-10.24
06/11/10-06/22/11	50.00	33.68	18.12	16.77	0.75	0.59	1.33	1.68	2.20	2.15	2.59	2.80	11.09
06/22/11-05/15/12	0.00	18.08	18.48	21.23	0.22	0.33	1.44	1.18	1.19	1.01	2.58	2.43	-21.27
05/15/12-12/09/12	50.00	11.60	16.93	15.01	0.00	0.00	0.04	0.01	0.01	0.00	0.08	0.02	17.03
Total	150.00	117.97	93.20	86.57	1.46	1.53	4.56	4.51	4.70	4.70	8.12	8.17	31.07
Average	33.33	26.22	20.71	19.24	0.32	0.34	1.01	1.00	1.04	1.04	1.81	1.82	6.90

OBS, Observed; SIM, Simulated; ΔSP, Soil P change; DRP, Dissolved Reactive Phosphorus; PP, Particulate Phosphorus; GH, Grain Harvested.

3.3.4 Particulate Phosphorus (PP) Loss

Simulated PP loss through runoff and tile drainage agreed well with the observed data. Simulation results and statistics are presented in Figures 3.5c & 3.5d and Table 3.7, respectively. Analysis of observed data revealed that 68.09% of the net P loss (DRP+PP) was lost in the form of PP and tile drainage contributed (63.47% of the total PP loss) more PP loss than the surface runoff (Table 3.9). The model captured this well and simulated 68.04% of the net P loss in the form of PP and simulated tile drainage PP loss was 63.50% of the total PP loss. Overall, the model's ability in simulating PP loss through surface runoff and subsurface drainage was very good and good respectively. (Figure 3.5c, Figure 3.5d and Table 3.7).

3.3.5 Sum of DRP and PP (SumP) Loss

The simulation results of the sum of DRP and PP loss (SumP) through surface runoff and tile drainage) and its statistics are presented in Figures 3.5e, 3.5f & 3.5g and Table 3.7 respectively. Observed data revealed that tile drainage dominated the SumP loss composing 67.14% of total annual SumP loss while the simulated SumP loss through tile drainage was 67.46% of the total annual SumP loss. The simulation of SumP loss through surface runoff was very good (NSE >0.75, PBIAS within ± 25% and IoA > 0.75) while it was good during the validation period (NSE >0.65, PBIAS within ± 25% and IoA > 0.75). The simulation of SumP loss tile drainage during the calibration and validation period was good and very good respectively. Overall, the SumP loss simulations through both surface runoff and tile drainage were very good (Table 3.7). The simulation of total SumP loss from the field, such as sum of DRP in both runoff and drainage and PP in both runoff and drainage for the entire simulation period was also very good (Figure 3.5g and Table 3.7).

3.4 DISCUSSION

The field experiment showed that subsurface drainage was the major pathway of P loss from the field, comprising 67.14% of total annual average SumP loss. The annual average SumP loss through tile drainage was dominated by PP which accounted for 64.53% of total annual average SumP loss through tile drainage (Table 3.9). In contrast, a study conducted by Qi et al., (2017) with the ICECREAM model at the same site reported that ICECREAM failed to simulate the PP loss through tile drainage and that soil moisture content was also not simulated satisfactorily. They concluded that it could be improved by adopting the soil matric potential-based Richards equation to simulate soil matrix flow. Radcliffe et al., (2015) noted that, although ICECREAM was one of the best P simulation models available to date, it lacked macropore and tile drainage components.

The newly developed P model combined with RZWQM2 addressed all the concerns that were previously highlighted. Qi et al., (2017) reported that ICECREAM simulated DRP loss through tile drainage within 18% of observed values and with NSE of 0.66 while it failed to simulate PP loss through tile drainage (NSE <0.0 and PBIAS 44%). While comparing the simulation results of this study (Table 3.7) with those of Qi et al., (2017), we found that the P model's capability was particularly improved in its simulation of P losses through the tile drainage system. The model's simulation of P losses particularly through tile drainage system improved after the proper calibration of soil moisture. The adoption of Richards's equation led to better soil moisture and soil matrix flux simulations (Table 3.6). This had a direct impact on P dynamics, as soil moisture governs the decomposition and mineralization rate and P flows among the various pools and soil matrix flux determines the amount of P loading to the tile drainage system. The use of Poiseuille's law resulted in better macropore flow simulations, which is one of the major pathways of DRP and PP loading to the tiles. Finally, the use of Hooghoudt's steady state equation further improved tile drainage simulations and P loss through tile drainage. Soil temperature also has an important role in simulation of P dynamics in agricultural fields. An acceptable soil temperature simulation (Table 3.6) led to good estimation of P flow rate among various P pools, decomposition and mineralization rates of residue and soil organic matter.

Analysis of the observed data for both growing seasons (periods 2-3, 7-8, 11-12, 15-17, 19) and non-growing seasons (periods 1, 4-6, 9-10, 13-14) revealed that 75.71% of total drainage volume and 60.14% of total runoff volume occurred in the non-growing seasons. Consequently, the P loss during non-growing seasons was dominant. During non-growing seasons, runoff carried away 56.24% of the total runoff bound DRP, whereas 64.47% of total tile drainage-bound DRP loss occurred during non-growing seasons. The same was observed for the PP loss, with 64.97% of total runoff associated PP and 74.34% of total drainage associated PP being lost during the non-growing seasons. SumP loss in the non-growing seasons during the whole simulation years comprised 68.19% of total SumP loss through surface and subsurface water flow. The newly developed model satisfactorily simulated the fact that the major flow and P loss from the field occurred during non-growing seasons. For simulated discharge, 66.97 % of total runoff and 67.91% of total drainage occurred in the non-growing seasons whereas simulated SumP loss during non-growing seasons represented 65.76% of the total SumP lost through surface and subsurface water flow. These simulated results also corresponded well to the observations of King et al., (2015), who found that the non-growing period "represents a significant proportion of annual discharge and P loss".

The developed RZWQM2-P model is easy to run with menu driven graphical user interface. Although the data required to run the model seems to be meticulous, but it can be easily collected from many resources when in-situ measurement is not feasible. Weather data can be obtained from online resources for free or with nominal charges. Agricultural management data can be collected while interviewing the farmer or the farm manager of the site. It can also be made available from various factsheets as published time to time by various agricultural agencies. Soil data can be derived using basic county soil survey information along with pedotransfer functions (Schaap et al., 2001) or tables as provided by Ma et al., (2011) and Rawls et al., (1982). Initial soil P values can be estimated while running the model for certain amount of years prior to start of actual simulation year with typical agronomical management practices and cropping system of the site. RZWQM2-P has in built database of crop phenology parameters for most common crop cultivars. This database can be used to default the crop phenology parameters.

Computer simulation models inevitably have some limitations because they are built on assumptions and simplified version of the very complex real-world phenomenon. In this context RZWQM2-P model is limited to one dimensional and assuming soil as a homogeneous medium. The model is not designed to simulate dissolved unreactive P loss. It also assumes that PP originates from the first 0.01 m soil layer and only the macropore flow contribute to tile drainage bound PP loss. Another shortcoming of RZWQM2-P is that it is a field scale model, which cannot be applied over large-scale watershed. Despite these limitations and assumptions, RZWQM2-P can be used in a wide range of scenarios to mitigate P pollution under various agricultural management practices along with different cropping systems that are commonly adopted in North America. Agricultural management practices include tile drainage, control drainage with or without sub-irrigation, various type of tillage application, surface, sub-surface and injected inorganic fertilizer/manure application. Manure type includes poultry, swine, beef cattle and dairy cattle under solid and liquid phases. RZWQM2-P can also be applied to identify the impact of winter manure application, which is a common practice in many areas of North America.

In this present study we presented the development of RZWQM2-P and its very first evaluation with a tile drained corn soybean rotated field under inorganic P fertilization over a period of four and half years. The evaluation resulted in satisfactory performance of the model over the both calibration and validation periods. Although RZWQM2-P seems to be a promising tool to manage agricultural P under the given management practices, to be certain about the efficacy of the model further tests are recommended at several other locations under different fertilization (i.e. manure), soil, climate, and crop conditions for a longer period with more observational data.

3.5 CONCLUSIONS

In this study, a model based P management tool was developed to simulate the fate and transport of DRP and PP from an agricultural field based on most recent scientific findings while overcoming the limitations of the ICECREAM model as highlighted by previous researchers (Qi et al., 2017; Radcliffe et al., 2015), and taking advantage of the process-based agro-hydrologic model RZWQM2. The new P model incorporated into RZWQM2 combined the proven strengths in simulating the impacts of agricultural management practices and hydrological processes in an agricultural field with the ability to simulate P dynamics. The P model was evaluated against four and a half years of data collected from a subsurface-drained corn-soybean rotated field with clay loam soil in southwestern Ontario, Canada. The simulation results showed that the newly developed model performed satisfactorily in simulating the DRP and PP losses through both surface runoff and subsurface drainage with all periods NSE > 0.65, PBAIS within 25% and IoA > 0.75. The P model's P loss simulating ability was improved particularly through tile drainage by adopting Richards's equation for simulation of soil matrix flow, and Hooghoudt's equation for simulation of tile drainage flow. The use of Poiseuille's law may have resulted in better macropore flow simulations, which led to better simulations of PP loading to the tile system. However, this needs further investigations. The simulation results were consistent with the observed trend that the non-growing season dominated the P loss over growing seasons, tile drainage contributed more towards these losses, and PP was the major form of P loss. The newly developed P module integrated with RZWQM2 is a promising tool for P management, particularly for subsurface-drained fields. Further tests are needed to evaluate this model under different fertilization (manure), soil, climate, and crop conditions.

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CONNECTING TEXT TO CHAPTER 4

Chapter 3 presented the development and very first evaluation of the newly developed RZWQM2-P model. The evaluation revealed satisfactory performance of the model's simulation of P losses both through surface runoff and tile drainage under inorganic fertilizer application. The Chapter 4 presents another evaluation and application of the newly developed P model (RZWQM2-P) (Root Zone Water Quality Model-Phosphorus) under manure application. The model was evaluated against the measured dataset including subsurface tile drainage, surface runoff, DRP and PP loss through tile drainage and surface runoff, soil water content, soil temperature from a corn soybean rotated, artificially drained experimental field. After the evaluation, the calibrated model was subsequently applied to identify the best management strategy to mitigate P losses from the field.

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1. Department of Bioresource Engineering, McGill University, Sainte-Anne-de-Bellevue, Quebec, H9X 3V9, Canada

2. Harrow Research and Development Center, Agriculture and Agri-Food Canada, Harrow, Ontario, N0R 1G0, Canada

3. USDA-ARS Rangeland Resources and Systems Research Unit, Fort Collins, Colorado, 80526, USA.

CHAPTER 4

MODELING AND MITIGATING PHOSPHORUS LOSSES FROM A TILE-DRAINED AND MANURED FIELD USING RZWQM2-P

Debasis Sadhukhan[1], Zhiming Qi[1*], Tie-Quan Zhang[2], Chin S. Tan[2], Liwang Ma[3]

1. Department of Bioresource Engineering, McGill University, Sainte-Anne-de-Bellevue, Quebec, H9X 3V9, Canada

2. Harrow Research and Development Center, Agriculture and Agri-Food Canada, Harrow, Ontario, N0R 1G0, Canada

3. USDA-ARS Rangeland Resources and Systems Research Unit, Fort Collins, Colorado, 80526, USA.

ABSTRACT

Prediction of phosphorus (P) losses from manured agricultural fields through surface runoff and tile drainage is necessary to mitigate widespread eutrophication in water bodies. However, present water quality models are weak in predicting P losses particularly in tile drained and manure applied cropland. We developed a field scale P management model RZWQM2-P whose accuracy in simulating P losses from manure applied agricultural field is yet to be tested. The objectives of this study were 1) to assess the accuracy of this new model in simulating dissolved reactive phosphorus (DRP) and particulate phosphorus (PP) losses in surface runoff and tile drainage from a manure amended field; and 2) to identify best management practices to mitigate manure P losses including water table control, manure application timing and spreading methods by the use of model simulation. The model was evaluated against data collected from a liquid cattle manure applied field with corn-soybean rotation in Ontario, Canada. The results revealed that the RZWQM2-P model satisfactorily simulated DRP and PP losses through both surface runoff and tile drainage (NSE > 0.50, PBAIS within ± 25% and IoA > 0.75). Compared to conventional management

practices, manure injection reduced the P losses by 18% whereas controlled drainage and winter manure application increased P losses by 13% and 23%, respectively. The RZWQM2-P is a promising tool for P management in manured and subsurface drained agricultural field. The injection of manure rather than controlled drainage is an effective management practice to mitigate P losses from a subsurface drained field.

4.1 INTRODUCTION

Non-point source phosphorus (P) pollution of surface water bodies originating from the upstream agricultural lands are becoming a serious environmental concern, degrading the water quality and causing rapid increase in algal population and eutrophication (Guildford and Hecky, 2000). Sources of P in an agricultural field mostly are soil, plant materials and applied fertilizer and manure (Hansen et al., 2002; Heathwaite and Dils, 2000; Withers et al., 2001). Among these the greatest potential for accelerated P losses occur with manure application (Duda and Finan, 1983; Eghball and Gilley, 1999; Kleinman and Sharpley, 2003; Moore et al., 2000). Almost all manure produced on Canadian farms is applied to agricultural land (Patni, 1991). In Ontario, animal husbandry generates approximately 16 million cubic meters of liquid manure and 22 million tons of solid manure, which are mainly applied to large areas of farmland (OMAFRA, 2005). Based on Statistics Canada data, the area of manure application was approximately 2.83 Mha (4% of total agricultural area) in whole Canada while in Ontario 0.75 Mha (15 % of total agricultural area) and 0.85 Mha (26 % of total agricultural area) in Quebec was manure applied during the year 2016. As a primary control of surface water eutrophication, P losses from manured soils have prompted a broad array of guidelines and regulations (USEPA, 1996; OMAFRA, 2002).

In northern US and eastern Canada, winter manure application is fairly common and had several advantages. For example, it nullifies the use of manure storage structures, allows more spreading time and reduce soil compaction (Srinivasan et al., 2006) but at the same time, it is prone to more nutrient loss (Liu et al., 2018, 2017a; Vadas et al., 2017) as compared to spring manure application. However, because of frozen soil, winter applied manure normally could not be incorporated and due to nutrient losses under frequent runoff from snowmelt and rain on snow events, governments have restricted winter manure application to prevent loss of manure constituents including P (Srinivasan et al., 2006). Because of limited number of studies on quantifying nutrient losses from manure upon winter application, these government restrictions on winter manure spreading are based more on commonly held perceptions rather than on research (Srinivasan et al., 2006). Therefore, a modeling approach can be employed to quantify the effect of winter manure application on P losses.

Agricultural subsurface tile drainage is a commonly used management practice in many parts of the USA and Canada to improve the soil's natural drainage and subsequently to increase crop yield (Evans et al., 1995). Unfortunately, tile drainage can also increase mobile nutrient losses with subsurface flow (Tan et al., 1993, 1998, 2002b ; Rudolph and Goss 1993; Ruark et al., 2012; Zhang et al. 2015b) as it tends to increase total water yield from an agricultural field. This increased nutrient loading pollutes surface and groundwater resources. A modification of subsurface drainage system, which uses a riser on tile outflows, known as controlled drainage, is now being used in order to prevent excessive drainage and subsequently nutrient losses. Research indicates that controlled drainage reduced tile drainage water volume (Tan et al., 2002a) and nitrate-N loss over conventional tile drainage system (Drury et al., 2009; Fogiel and Belcher 1991; Tan et al., 1998). For P losses there are a few studies which investigated this and they were contradictory. Valero et al., (2007) and Stämpfli and Madramootoo (2006) found that controlled drainage system was not effective to reduce P losses whereas Tan and Zhang (2011) and Zhang et al., (2015b) found that controlled drainage reduced P losses from an agricultural field.

Nutrient losses are aggravated by conventional surface broadcast applications because the nutrients remain completely exposed to rain and runoff whereas subsurface injection is can be practiced to reduce nutrient losses from an agricultural field (Pote et al., 2006; Watts et al., 2011). However, modeling studies to substantiate this fact are limited.

Kleinman et al., (2015) indicated that computer modeling using measured P data was currently one of the priorities in improving one's understanding of P dynamics in an agricultural field in order to mitigate freshwater eutrophication. However, commonly used models such as EPIC (Williams et al., 1983), GLEAMS (Leonard et al., 1987), ANSWERS (Bouraoui and Dillaha, 1996) and ICECREAM (Tattari et al., 2001) do not have dedicated surface manure P pools to simulate P dynamics due to manure application (Pierson et al., 2001; Sharpley et al., 2002). There are also lack of models which can simulate P losses through tile drainage (Radcliffe et al., 2015) which is one of the major pathways of P loading from agricultural fields to freshwater bodies (Ruark et al., 2012; Tan and Zhang, 2011). Of available agricultural P management models, ICECREAM seems to be the best at simulating P losses through tile drains (Radcliffe et al., 2015). However, ICECREAM does not have a water table-based tile drainage simulation component. It uses a simple storage routing concepts to simulate matrix flow and macropore flow (Qi and Qi, 2016; Tattari et al., 2001) and these fluxes at first contributes to a groundwater reservoir then from the groundwater reservoir tile flow get initiated when the storage capacity defined by a user defined threshold value is exceeded (Larsson et al., 2007). This conceptual approach is reported to be less accurate (Larsson et al., 2007). This may be improved by adopting the soil matric potential based Richard's equation (Richards, 1931) to simulate matrix flow, Poiseuille's law based approach to simulate macro pore flow and Hooghoudt's equation (Bouwer and Schilfgaarde 1963) to simulate tile drainage.

Root Zone Water Quality Model 2 (RZWQM2, Ahuja et al., 2000) is a field-scale one dimensional agricultural process control model which is widely applied in simulating the impacts of agricultural management practices on hydrology, water quality, crop growth, and greenhouse gas emission at locations across the United States (Ma et al., 2004,2007a,b; Qi et al., 2011,2013) Canada (Ahmed et al., 2007 a,b; Jiang et al., 2018) and in China (Fang et al., 2010 , 2013; Liu et al., 2017b) but it lacked a P subroutine. We developed a P module for the RZWQM2 model (RZWQM2-P, Sadhukhan et al., 2019a) to simulate P dynamics, based on scientific findings regarding the fate and transport of P from tile drained agricultural field. The developed RZWQM2-P is capable of simulating dissolved reactive P (DRP) and particulate P (PP) loss through both tile drainage and surface runoff under inorganic P application (Sadhukhan et al., 2019a) but its capability to simulate P losses under manure application is yet to be tested. Further, the impacts of agricultural management practices, such as controlled drainage, winter manure application and manure injection, on P losses are needed to be quantified. Therefore, in this study we calibrated and validated the newly developed RZWQM2-P model against measured hydrologic and P data in a tile drained field with liquid cattle manure application and corn-soybean rotation and subsequently applied the calibrated model to quantify the impacts of those agricultural management practices on P losses and to identify the most effective management practice among them to reduce P losses.

4.2 MATERIALS AND METHODS

4.2.1 RZWQM2-P Model Overview

Developed by the USDA-ARS, the RZWQM2 model (Ahuja et al., 2000) is a field scale, one dimensional agricultural process control model with daily time step. The model employs the Richards equation (Richards, 1931) to simulate soil water redistribution within the soil profile following infiltration which is simulated by the Green-Ampt method (Green and Ampt, 1911). Surface runoff is generated when the rainfall rate exceeds the infiltration rate and sediment yield is computed using USLE method (Wischmeier and Smith, 1978). Tile drainage flow is calculated by Hooghoudt's steady state equation (Bouwer and Schilfgaarde, 1963) and the macropore flow is governed by the Poiseuille's law. The crop growth can be simulated either by embedded DSSAT 4.0 crop models (Jones et al., 2003) or a generic crop production model (Hanson, 2000) whereas evapotranspiration is estimated using the double layer Shuttleworth-Wallace model (Shuttleworth and Wallace, 1985). The P model within RZWQM2 model is designed with five different soil P pools: three inorganics, namely labile P (LabP), active inorganic P (ActIP) and stable inorganic P (StabIP) and two organic pools namely fresh organic P pool (FresOP)and stable organic P pool(StabOP) respectively, following the nomenclature of Jones et al., (1984). Besides these soil P pools, as an advanced feature the model also has four surface manure P pools and two surface fertilizer P pools to simulate P dynamics arising from the application of fertilizer and manure (Vadas et al., 2004, 2007, 2008; Vadas, 2014). The manure P pools are inorganic water extractable P (ManWIP), inorganic stable P (ManSIP), organic water extractable P (ManWOP), and organic stable P (ManSOP). The fertilizer P pools were available fertilizer P (AvFertP) and residual fertilizer P (ResFertP) pool. Among these P pools, plant can uptake P for its growth from the LabP pool only and it is considered to be in dissolved form. The simulation of plant P uptake is based on Neitsch et al., (2011). The absorption and desorption of P among the inorganic soil P pools is simulated based on Jones et al., (1984) with advanced dynamic absorption and desorption rate as prescribed by Vadas et al., (2006). Mineralization and immobilization of P is simulated based on Jones et al., (1984). Mineralization and immobilization of P is simulated based on Jones et al., (1984) while the P decomposition rate from plant residue and soil humus is assumed to be the same as carbon decomposition which is simulated based on Shaffer et al., (2000). Applied manure P is distributed within the surface manure pools based on application depth, type and properties of manure applied. For the liquid manure application, 60% of the applied manure P immediately infiltrates into the soil added to the soil P pools of the top most soil layer (LabP, ActIP) (Vadas et al., 2007). Leached and decomposed P from the manure P pools are added to the soil P pools. The RZWQM2-P model simulates tile drainage bound DRP and PP loss following Francesconi et al., (2016) and Jarvis et al., (1999) respectively. The model assumes that particle bound P originates from the first soil layer of the soil profile and PP through soil profile is only transported through the macropore flow and contributes directly to the tile system bypassing the soil matrix. In the model DRP and PP loss through surface runoff is simulated as per Neitsch et al., (2011) and McElroy et al., (1976) respectively. LabP and two manure water extractable P pools contribute to DRP loss whereas all the P pools contribute to PP loss. The processes of P movement among the fertilizer, manure, organic and inorganic P pools and plant P uptake are described with greater details in Sadhukhan et al., (2019a). While the P model simulates P dynamics, the RZWQM2 governs the physical, biological, chemical and hydrological processes that influence the P simulation i.e. crop growth, runoff, drainage, soil moisture and its flux, soil temperature, sediment yield, macropore flow, plant residue and soil humus decomposition and agriculture management practices such as tillage. All these components are simulated by RZWQM2 within its original functionalities and then the P model uses them to simulate P dynamics and P losses through surface runoff and tile drainage.

4.2.2 Field Experiment

The RZWQM2-P model was assessed against observed DRP and PP loss in both surface runoff and tile drainage water flow from the Hon. Eugene F. Whelan Research Farm near South Woodslee, ON (42.21N, 82.74W) for eight cropping years from June 2008 to April 2016. The site was comprised of 16 plots (67.1 m × 15.2 m) receiving different fertilizer types and drainage treatments. Among these, plot number 4 and 14, were selected for the present study. These plots received liquid cattle manure application and were subject to tile drainage (depth: 0.85 m, spacing: 3.80 m). The crop was rotated between maize (*Zea mays L.*) and soybean (*Glycine max (L). Merr*.) in alternating years. In even years maize was planted at a density of 79,800 seeds ha^{-1}, while in odd years soybean was planted at a density of 486,700 seeds ha^{-1}. The liquid cattle manure equivalent to 50 kg P ha^{-1} and 200 kg N ha^{-1} were surface-applied in the year 2008, 2010, 2012 and 2014 before maize planting. Manure water extractable P content was not measured, so we assumed that in liquid cattle manure 60% of total P was water extractable P (Kleinman et al., 2005). Chisel plow tillage was implemented each year before planting and after harvest. The dates of cropping and other management practices are presented in Table 4.1.

Table 4.1: Crop and management practices at the site

Management practices	2008	2009	2010	2011	2012	2013	2014	2015
Spring tillage	01-Jun	05-Mar	11-Jun	14-Jun	25-Apr	08-May	24-Apr	27-Apr
Manure application	02-Jun	-	12-Jun	-	16-May	-	24-Jun	-
Crop planting	18-Jun	22-May	26-Jun	15-Jun	25-May	16-May	29-Jun	25-May
Crop harvest	05-Nov	20-Oct	08-Nov	13-Dec	05-Nov	09-Oct	28-Nov	07-Oct
Fall tillage	18-Nov	01-Nov	19-Nov	20-Dec	19-Nov	29-Oct	02-Dec	20-Oct

The soil type was clay loam and the measured soil properties for plots 4 & 14 were averaged (Table 4.2) and used as the soil input data for the model. The soil profile was divided into six layers. The soil properties such as soil texture, field capacity (θ_{fc}), permanent wilting point (θ_{wp}) soil bulk density (ρ) and porosity (φ) were measured before the start of the experiment. Prior to the onset of the experiment in 2008, soil labile P was measured using the Olsen P method (Olsen et al., 1954) while soil total P was measured following the soil testing recommendations by OMAFRA (2009). During growing seasons from 2010 onwards volumetric soil moistures (θ) for the soil layer between 0-80 mm was measured twice a week using a portable TDR probe, while soil temperature (T_{soil}) at a depth of 50 mm was measured on an hourly basis using sensors. Hourly T_{soil} were averaged to obtain daily mean T_{soil}.

Table 4.2: Measured and calibrated soil properties.

	Measured soil properties									Calibrated soil properties			
Soil Layer depth (mm)	ρ (kg m^{-3}	Clay (%)	Sand (%)	OM (%)	θ_{fc} (m^3 m^{-3})	φ (m^3 m^{-3})	θ_{wp} (m^3 m^{-3})	LabP (g kg^{-1})	TotalP (g kg^{-1}	P_b (cm)	λ	K_{sat} (cm h^{-1})	K_{lat} (cm h^{-1})
0-10	1330	34.2	29.0	3.7	0.37	0.54	0.18	0.02	0.90	-20.06	0.16	0.01	0.02
10-100	1330	34.2	29.0	3.7	0.37	0.54	0.18	0.02	0.90	-29.03	0.15	0.35	0.70
100-250	1390	34.2	29.0	3.7	0.36	0.54	0.18	0.02	0.90	-16.64	0.20	0.55	1.10
250-450	1390	40.7	25.7	2.0	0.35	0.5	0.18	0.01	0.65	-16.16	0.19	0.55	1.10
450-800	1330	40.4	27.0	0.7	0.36	0.48	0.18	0.01	0.50	-25.10	0.15	0.17	0.35
800-1200	1330	39.3	24.6	0.5	0.36	0.48	0.17	0.01	0.40	-35.17	0.14	0.17	0.35

ρ, Soil bulk density; Clay, Soil clay content; Sand, Soil sand content; OM, Soil organic matter content; θ_{fc}, Volumetric soil moisture content at field capacity; φ, Soil porosity; θ_{wp}, Volumetric soil moisture content at permanent wilting point; pH, soil pH; LabP, Soil labile P, TotalP, Soil total P; P_b, Air entry pressure; λ, Pore size index; k_{sat}, Saturated hydraulic conductivity; k_{lat}, Lateral hydraulic conductivity;

The required weather data (air temperature, precipitation, relative humidity, solar radiation and wind speed) to run the model were collected for the period of 1st Jan. 2008 to 31st Dec. 2016 from the automated meteorological weather station located at the Whelan farm, located less than 500 m from the experimental plots. In each experimental plot there was a catch basin at their downstream end to collect the surface runoff. Surface runoff and tile drainage from the experimental plot were directed to a central instrumentation building via underground PVC pipes. In the instrumentation building, the flow rate was measured automatically using electronic flowmeters and recorded in a multi-channel data logger. Surface runoff and tile drainage were collected at the end of each plot automatically using autosamplers (CALPSO 2000S, Buhler Gmbh & Company). Surface and tile water samples were collected continuously (year-round), proportionally to flow volume, samples being taken for every 1000 L of flow during the growing season and for every 3000 L of flow during the non-growing seasons. After the collection the samples were analyzed in the laboratory for DRP and total dissolved P (TotalDP) using an acidified ammonium persulfate [$(NH_4)_2S_2O_2$] oxidation procedure (USEPA, 1983). Unfiltered water samples were analyzed for total P (TotalP) using the sulfuric acid-hydrogen peroxide digestion method (USEPA, 1983). The PP was computed by the difference between TotalP and TotalDP.

4.2.3 Model Calibration and Validation

The RZWQM2-P model was run using the eight crop years (June 2008 – April 2016) with the measured surface runoff and subsurface drainage and corresponding DRP and PP loss data as collected from the experimental site. Measured Olsen P values were used to initialize the LabP pool while all other inorganic and organic P pools were initialized based on this measured LabP values following Jones et al., (1984). All the manure and fertilizer P pools were initialed as zero. There were some limitations on flow event separation so to maintain reality of the P loss, water sample collecting periods were scheduled which resulted in total 34 different periods (Table 4.3) for the study period. Out of these 34 periods, the first nineteen periods (01 June 2008 to 09 Nov 2012) were randomly selected for calibrating the model whereas the last fifteen period (10 Nov 2012 to 31 April 2016) were selected for validating the model. During the calibration process, at first parameters related to soil moisture, surface runoff and tile drainage simulation were calibrated as these processes govern P loss from an agricultural field, then the parameters related to P losses were calibrated. The calibration was done manually by trial and error while changing one parameter at a time, within the range as obtained from available literature, following the methods as mentioned by Ma et al., (2011, 2012) for the hydrological calibration and Sadhukhan et al., (2019a) for P losses calibration. Three model evaluation statistics such as Nash-Sutcliffe efficiency (NSE), percent bias (PBIAS), and index of agreement (IoA) were used to evaluate the performance of the model in simulating hydrology, soil moisture, soil temperature and P losses through surface runoff and tile drainage based on the criteria presented in Moriasi et al., (2007, 2015). The NSE is a normalized statistic that determines the relative magnitude of the variance in simulated data as compared to the measured data and it is sensitive to peak values, the IoA is a standardized measure of the degree of model prediction error whereas PBAIS reflects the goodness of model's simulation in respect of the observed data. The model is regarded to perform satisfactorily when NSE > 0.50 and good when NSE > 0.65. Model performance is deemed to be satisfactory when |PBIAS| is between 15% and 25% for water flow and is between 40% and 70% for P and it is deemed to be good when |PBIAS| is between 10% and 15% for water flow and is between 25% and 40% for P (Moriasi et al., 2007). Model performance is regarded as acceptable when IoA > 0.75 (Moriasi et al., 2015).

Table 4.3: Periods of water flow and P measurement data for calibration and validation

Period no.	Period Calibration	Period no.	Period Validation
1	1/Jun/2008-16/Jun/2008	20	10/Nov/2012-15/Mar/2013
2	17/Jun/2008-17/Jul/2008	21	16/Mar/2013-23/May/2013
3	18/Jul/2008-22/Oct/2008	22	24/May/2013-26/Jun/2013
4	23/Oct/2008-11Feb/2009	23	27/Jun/2013-02/Aug/2013
5	12/Feb/2009-27/Mar/2009	24	03/Aug/2013-26/Mar/2014
6	28/Mar/2009-26/May/2009	25	27/Mar/2014-23/Jun/2014
7	27/May/2009-16/Jul/2009	26	24/Jun/2014-05/Aug/2014
8	17/Jul/2009-23/Oct/2009	27	06/Aug/2014-26/Nov/2014
9	24/Oct/2009-20/Apr/2010	28	27/Nov/2014-25/Mar/2015
10	21/Apr/2010-11/Jun/2010	29	26/Mar/2015-28/May/2015
11	12/Jun/2010-5/Aug/2010	30	29/May/2015-04/Jun/2015
12	6/Aug/2010-21/Dec/2010	31	05/Jun/2015-07/July/2015
13	22/Dec/2010-23/Mar/2011	32	08/July/2015-15/Oct/2015
14	24/0Mar/2011-22/Jun/2011	33	16/Oct/2015-17/Mar/2016
15	23/Jun/2011-07/Sept/2011	34	18/Mar/2016-29/Apr/2016
16	08/Sept/2011-07/Nov/2011		
17	08/Nov/2011-22/Dec/2011		
18	23/Dec/2011-15/May/2012		
19	16/May/2012-09/Nov/2012		

The soil moisture content simulation within RZWQM2 model is parametrized with air entry pressure (P_b) and pore size distribution index (λ). At the start of the simulation, the values of P_b and λ were defaulted as given by Ma et al., (2011) then subsequently these values were modified one at a time to match the observed values. Once the soil moisture content was calibrated then calibration of runoff and tile drainage followed. In the model runoff is simulated when the rainfall rate exceeds the infiltration rate (Ma et al., 2012), so the parameters such as saturated hydraulic conductivity (k_{sat}) of the top soil layer and surface crust hydraulic conductivity (k_{crust}) were adjusted to calibrate runoff. Furthermore, the albedo was adjusted for simulation of evapotranspiration, which in turn affected surface runoff. For tile drainage calibration, parameters such as k_{sat}, P_b , lateral hydraulic conductivity (k_{lat}) and macroporosity were adjusted. k_{lat} had very prominent influence in tile drainage simulation and it was adjusted to $2 \times k_{\mathrm{sat}}$. In addition, P_b was slightly adjusted to better match tile drainage without hampering the previous calibration for soil moisture. The DRP loss through surface runoff was calibrated by adjusting the soil P extraction coefficient while DRP loss through tile drainage calibration depended on macroporosity, P_b and λ of the deeper soil layers. To control the DRP loading to the tile by macropore flow, the macroporosity value was adjusted and subsequently the P_b and λ of the deeper soil layers were slightly adjusted to control the DRP loading to tile by matrix flow without hampering previous calibration of tile drainage and soil moisture simulations. The PP loss through surface runoff was calibrated by adjusting USLE soil loss coefficients (soil erodibility factor, cover and management factor, support practice factor) and Manning's n ' for the overland flow profile segment while the PP loss through tile drainage is governed by parameters like soil replenishment rate coefficient, soil detachability coefficient, soil filtration coefficient and macroporosity. All these parameters were carefully balanced to get a reasonable simulation with respect to PP loss through tile drainage. At last, to control the plant P uptake from the LabP pool, the P uptake distribution parameter for each crop was adjusted. This parameter controls the depth distribution of the plant P uptake within the soil profile. Higher the values of P uptake distribution parameter, more amount of P is up taken by the plant from the topsoil layers. Calibrated soil hydraulic parameters and their values are presented in Table 4.2 and all other calibrated parameters are presented in Table 4.4.

Table 4.4: Calibrated parameters and their values

Parameters	Calibrated values	Default (Range)
Surface Crust (K_{crust})(cm hr^{-1})	0.01	0.01 (0.01-20.00)
Albedo		
Dry soil	0.75	0.20 (0.01-0.90)
Wet Soil	0.85	0.30 (0.02-0.90)
Crop at Maturity	0.55	0.70 (0.01-0.90)
Fresh Residue	0.85	0.22 (0.01-0.90)
Macroporosity (m^3 m^{-3})	0.03	-
P extraction coefficient (-)	1.00	1.00 (0.10-1.00)
USLE Coefficients		
Soil erodibility (t ha^{-1})	1.61	0.05 (0.01-1.97)
Cover and management factor	0.55	0.50 (0.01-1.00)
Support practice factor	0.55	0.50 (0.01-1.00)
Manning's n	0.01	0.01 (0.01-0.40)
Soil filtration coefficient (m^{-1})	0.20	0.00 (0.00-1.00)
Soil detachability coefficient (g J^{-1} mm^{-1})	0.60	0.40 (0.00-1.00)
Soil replenishment rate coefficient (gm m^{-2} day^{-1})	0.01	0.20 (0.00-1.00)
P uptake distribution parameter		
Corn	10.00	1.00-15.00
Soybean	10.00	1.00-15.00

4.2.4 RZWQM2-P Application

After the RZWQM2-P model was calibrated and validated, it was run to evaluate the impacts of controlled drainage, winter manure application and injected manure application on P losses under the same agro-climatic situation and for the same simulation period. For a controlled drainage system, the head gate at a depth of 460 mm from the ground level was maintained throughout the simulation period. To simulate winter manure application, each day during the non-growing periods (1st Jan – 15th May) of the corn planting years was selected as the application date. It resulted in total 136 simulations. P losses of all these simulations were subsequently averaged to identify average P losses under winter manure application. Finally, for injected manure application, the liquid cattle manure was assumed to be injected at a depth of 100 mm. For all these cases other agricultural management operations, manure properties kept exactly the same as the original simulation. The simulated P losses of these three management practices were then compared with original simulation with pre-planting manure application, which is generally the conventional management practices, to identify the best management practice to reduce P losses from the field.

4.3 RESULTS

4.3.1 Soil Moisture and Soil Temperature

Simulated and observed average soil moisture (θ) between 0-80 mm depths and soil temperature (T_{soil}) at 50 mm depth along with the simulation statistics for the calibration and validation periods are presented in Figure 4.1a and 4.1b, respectively. The model satisfactorily simulated θ during calibration period whereas in validation period it was simulated with NSE less than 0.50 (NSE =0.47) which is unsatisfactory but overall during the whole simulation period the model's simulation of θ was satisfactory with NSE 0.50, PBAIS 0.45% and IoA 0.81. T_{soil} simulation was satisfactory during calibration and validation period (Figure 4.1b). During the whole simulation period simulation of T_{soil} was also satisfactory with NSE 0.54, PBAIS 12% and IoA 0.89.

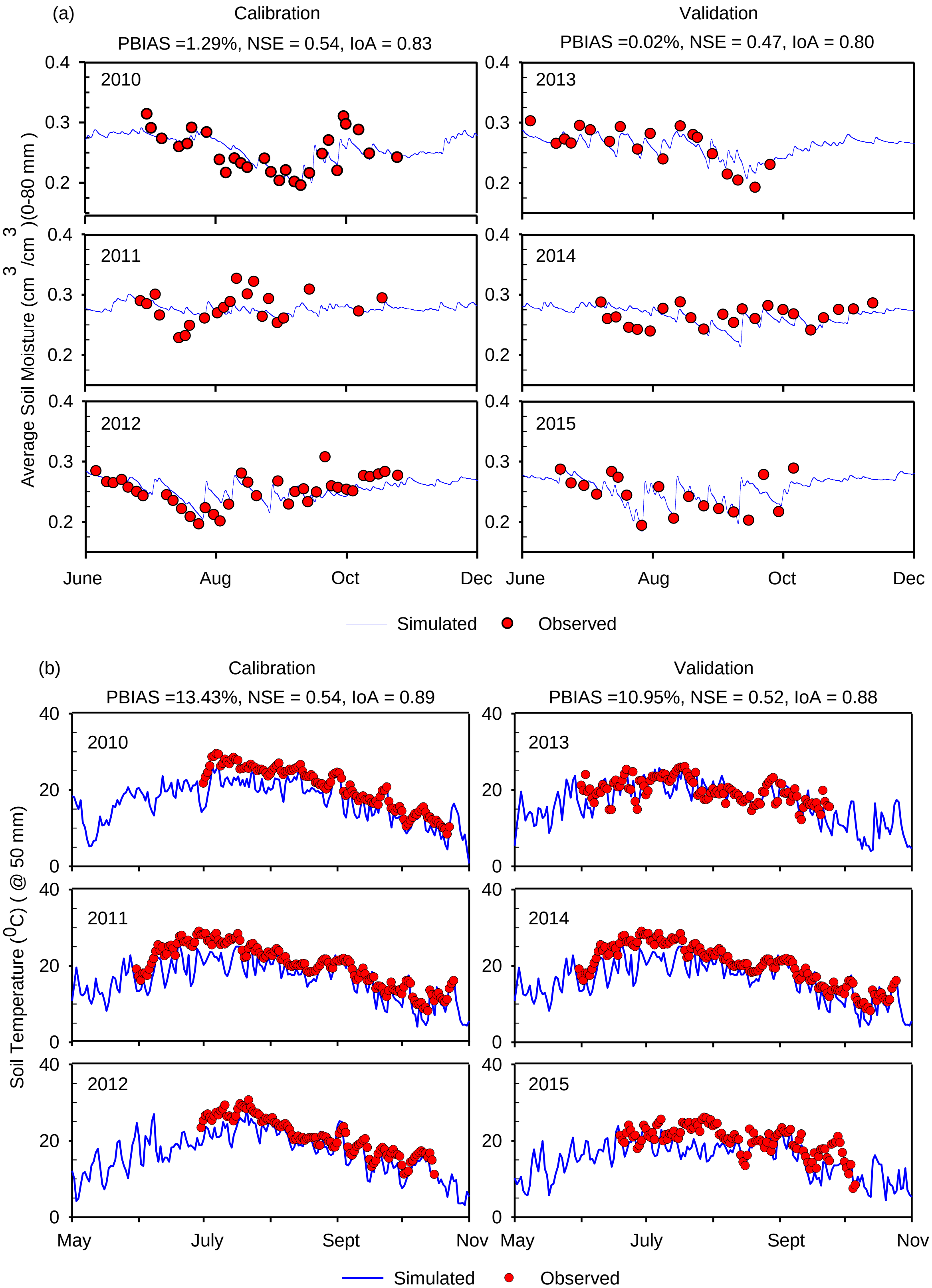

Figure 4.1: Simulated and observed (a) Average soil moisture (0-80 mm) (θ) and (b) Soil temperature (@ 50 mm) (T_{soil})

PBIAS, Percent bias, NSE, Nash-Sutcliffe model efficiency; IoA, Index of agreement.

4.3.2 Hydrology

Overall, the model's performance was very good in simulating runoff with NSE 0.80, PBAIS -3% an IoA 0.95 and was good in simulating tile drainage with NSE 0.67, PBAIS 10% an IoA 0.90. During the calibration period, simulated runoff showed (Figure 4.2a) high NSE value (NSE = 0.83), so did simulated tile drainage (Figure 4.2b) (NSE = 0.70) which is very good and good respectively according to Moriasi et al., (2007, 2015). On an annual basis, simulated average runoff and tile flow were close to the observed annual mean values (Table 4.5). During the eight years of simulation, simulated average annual ET (383 mm) was 42 % of the observed annual precipitation (910 mm). This was similar to measured annual ET of 45 % of the precipitation in the same region reported in Tan et al., (2002b). Between the simulated average annual surface runoff and tile drainage, most of the water (68%) moved out of the field through the tile drainage system.

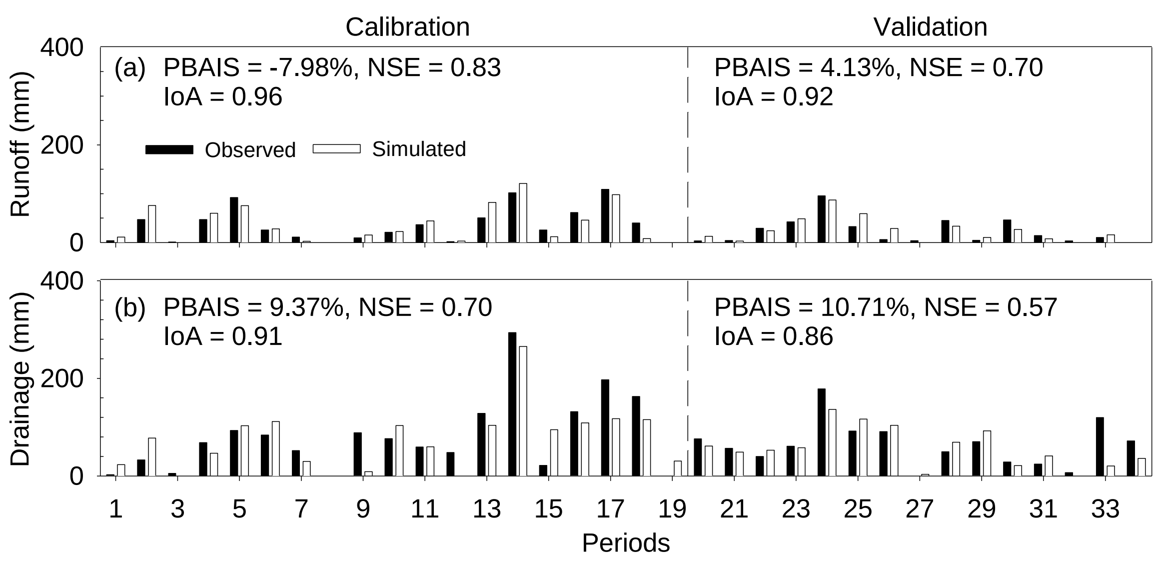

Figure 4.2: Simulated and observed (a) Runoff (b) Drainage.

PBIAS, Percent bias, NSE, Nash-Sutcliffe model efficiency; IoA, Index of agreement.

Table 4.5: Water balance table for the simulation period. All values are in mm

Year	Rainfall	ET	Runoff		Drainage		ΔS	Lateral Flow	Deep Seepage
	OB	SIM	SIM	OB	SIM	OB			
06/01/08-05/26/09	1113.90	386.17	249.56	215.97	361.36	286.03	-4.01	96.02	8.69
05/26/09-06/11/10	721.20	433.88	39.85	41.59	141.92	217.04	13.19	84.69	3.43
06/11/10-06/22/11	1171.50	349.49	249.68	190.44	428.82	529.16	18.47	100.59	12.26
06/22/11-05/15/12	995.30	309.61	163.61	235.25	436.50	513.42	-21.59	39.99	6.09
05/15/12-05/23/13	638.80	377.14	15.52	7.49	140.68	132.39	6.05	98.02	0.78
05/23/13-06/23/14	1207.67	498.48	218.15	198.98	363.84	370.92	-7.29	114.78	0.00
06/23/14-05/28/15	780.75	310.64	72.14	59.11	268.26	210.90	0.58	99.08	0.00
05/28/15-04/29/16	652.97	398.67	49.91	73.92	119.29	251.23	-15.64	95.49	0.00
Total	7282.09	3064.08	1058.41	1022.75	2260.66	2511.10	-10.24	728.66	31.25
Average (mm year^{-1})	910.26	383.01	132.30	127.84	282.58	313.89	-1.28	91.08	3.91

OBS, Observed; SIM, Simulated; ET, Evapotranspiration; ΔS, Soil water change

4.3.3 DRP and PP Loss

The performance of the RZWQM2-P in simulating P loss in terms of DRP and PP through surface runoff and tile drainage from a manured agricultural field can be judged as satisfactory (Figure 4.3). Model simulation suggested that DRP losses through surface runoff (Figure 4.3a) is driven by runoff volume, amount of P in LabP pool of the topmost soil layer and surface ManWIP pool. The model simulated annual average DRP loss (Table 4.6) is 0.29 kg P ha^{-1} and applied manure P contributed 5% of it, meaning that most of the simulated DRP in runoff came from soil P. This conforms to the idea that soil P is an important source of DRP loss through runoff (Wang et al., 2018a). The model simulated average annual DRP loss through tile drainage is 0.53 kg P ha^{-1} (Table 4.6) which is 83% more than simulated surface runoff associated DRP loss. This substantiate the model's assumption that in case of liquid manure application 60% of the applied P immediately infiltrates into the soil as soon as it is applied. This reduces the availability of manure P on the soil surface to be lost through surface runoff but increases DRP loss through tile drainage. The model's simulation suggested that macropore flow is the primary mechanism responsible for the DRP loss through tile drainage and it contributed 82% of the total DRP load of tile flow. Overall, the simulated DRP loss both through surface runoff and tile drainage closely flows the observed pattern with NSE 0.68, PBIAS 6% and IoA 0.93 for surface runoff and NSE 0.64, PBAIS 0.11% and IoA 0.89 for tile drainage. The simulation identified that 65% of total DRP loss was through tile flow, which conform to the observed fact that tile flow is the major pathway of the DRP loss from the experimental plot (Table 4.6). The simulation of PP loss through surface runoff and tile drainage in both calibration and validation period agreed well with the observed data (Figure 4.3c & 4.3d). The field experiment showed that 74 % of the total P was lost in the form of PP and tile drainage and surface runoff almost equally contributed towards this loss (Table 4.3). The model's simulation captured this satisfactorily with 75 % of total simulated P loss was in the form of PP and simulated tile drainage PP loss was half of the total PP loss. This also agrees with the observation of Tan and Zhang (2011), who reported that PP loss accounted majority of total P loss from a tiled drained agricultural field. The model successfully simulated total P loss through both the transport pathways from the field, i.e. the sum of DRP and PP in both runoff and drainage, with high simulation accuracy (NSE 0.86, PBAIS -0.46 % and IoA 0.96).

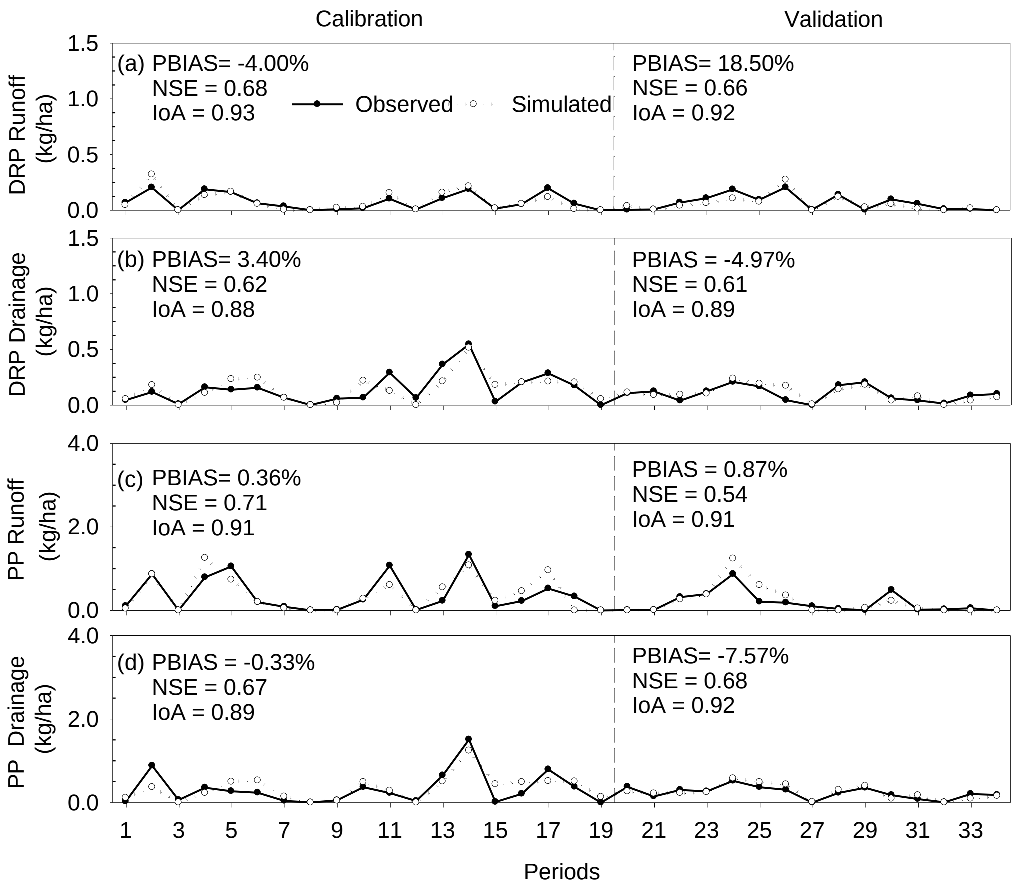

Figure 4.3: Simulated and observed (a) DRP in runoff (b) DRP in drainage, (c) PP in runoff and (d) PP in drainage.

PBIAS, Percent bias; NSE, Nash-Sutcliffe model efficiency; IoA, Index of agreement; DRP, Dissolved Reactive Phosphorus; PP, Particulate Phosphorus.

Table 4.6: P balance table for the simulation period (all values in kg ha^{-1})

Year	Manure P	Residue & Humus P Release	Plant Harvested	Grain Harvested	DRP Runoff		DRP Drainage		PP Runoff		PP Drainage		ΔSP
		SIM	SIM	SIM	SIM	OBS	SIM	OBS	SIM	OBS	SIM	OBS	SIM
06/01/08-05/26/09	50.00	27.67	51.44	18.25	0.70	0.68	0.81	0.62	2.81	3.02	1.71	1.83	18.34
05/26/09-06/11/10	0.00	25.96	36.39	21.21	0.05	0.06	0.30	0.19	0.31	0.36	0.66	0.46	-13.51
06/11/10-06/22/11	50.00	26.69	48.65	18.58	0.53	0.41	0.83	1.26	2.15	2.64	1.98	2.42	12.34
06/22/11-05/15/12	0.00	14.13	32.27	18.73	0.20	0.32	0.77	0.69	1.58	1.18	1.89	1.39	-26.16
05/15/12-05/23/13	50.00	21.42	51.38	16.54	0.04	0.01	0.25	0.23	0.01	0.02	0.60	0.52	28.27
05/23/13-06/23/14	0.00	22.82	34.73	19.80	0.28	0.45	0.61	0.54	2.39	1.79	1.49	1.46	-22.71
06/23/14-05/28/15	50.00	22.18	47.92	11.05	0.43	0.35	0.49	0.43	0.40	0.33	1.11	0.89	28.77
05/28/15-04/29/16	0.00	22.39	38.53	19.89	0.09	0.18	0.22	0.30	0.26	0.58	0.50	0.65	-8.86
Total	200.00	183.26	341.31	144.04	2.32	2.46	4.27	4.27	9.90	9.90	9.94	9.62	16.48
Average	25.00	22.91	42.66	18.01	0.29	0.31	0.53	0.53	1.24	1.24	1.24	1.20	2.06

OBS, Observed; SIM, Simulated; ΔSP, Soil P change; DRP , Dissolved reactive phosphorus; PP, Particulate phosphorus; P, Phosphorus;

The RZWQM2-P simulation results were in a good agreement with the observed fact that P loss was dominant during non-growing season in the experimental field. In this present study observed data showed that non-growing seasons (Dec to May) produced 68 % of total drainage volume and 58 % of total runoff volume. Subsequently runoff carried away 53% of the total runoff-bound DRP and 68% of total tile drainage-bound DRP during non-growing seasons. The same was observed for the PP loss, with 56% of total runoff associated PP and 65% of total drainage associated PP being lost during the non-growing seasons. P loss in the non-growing seasons during the whole simulation years comprised 61% of total P loss through surface and subsurface water flow. The RZWQM2-P simulated 61 % of total runoff and 65% of total drainage during the non-growing seasons whereas simulated P loss during non-growing seasons represented 65% of the total P lost through surface and subsurface water flow. These simulated results also corresponded well with the review report of King et al., (2015), who reported that the “non-growing period represents a significant proportion of annual discharge and P loss.

4.3.4 RZWQM2-P Application

Impact of three different agricultural management practices (controlled drainage, winter manure application, injected manure application) on P losses as identified by the simulation of RZWQM2-P and its comparison with conventional management practices are presented in Figure 4.4. Implementation of controlled drainage reduced the average annual tile flow volume (85%) whereas it increased average annual runoff volume (171%) over conventional management practices. Although controlled drainage reduced both DRP and PP loss through tile drainage (both 83%) but overall it increased (13%) total P loss because significant increase in surface runoff volume led to more runoff associated DRP and PP loss (188% and 110% respectively). Winter manure application simulation suggested increase in DRP and PP losses through both the transport pathways particularly DRP loss through surface runoff (63%) and overall it contributed 23% more total P loss as compare to conventional management practices. Simulation of injected manure application revealed as it is the best management practice among these three as it reduced DRP and PP losses both through surface runoff and tile drainage, thus as a whole it contributed to less total P loss (17%) from the field.

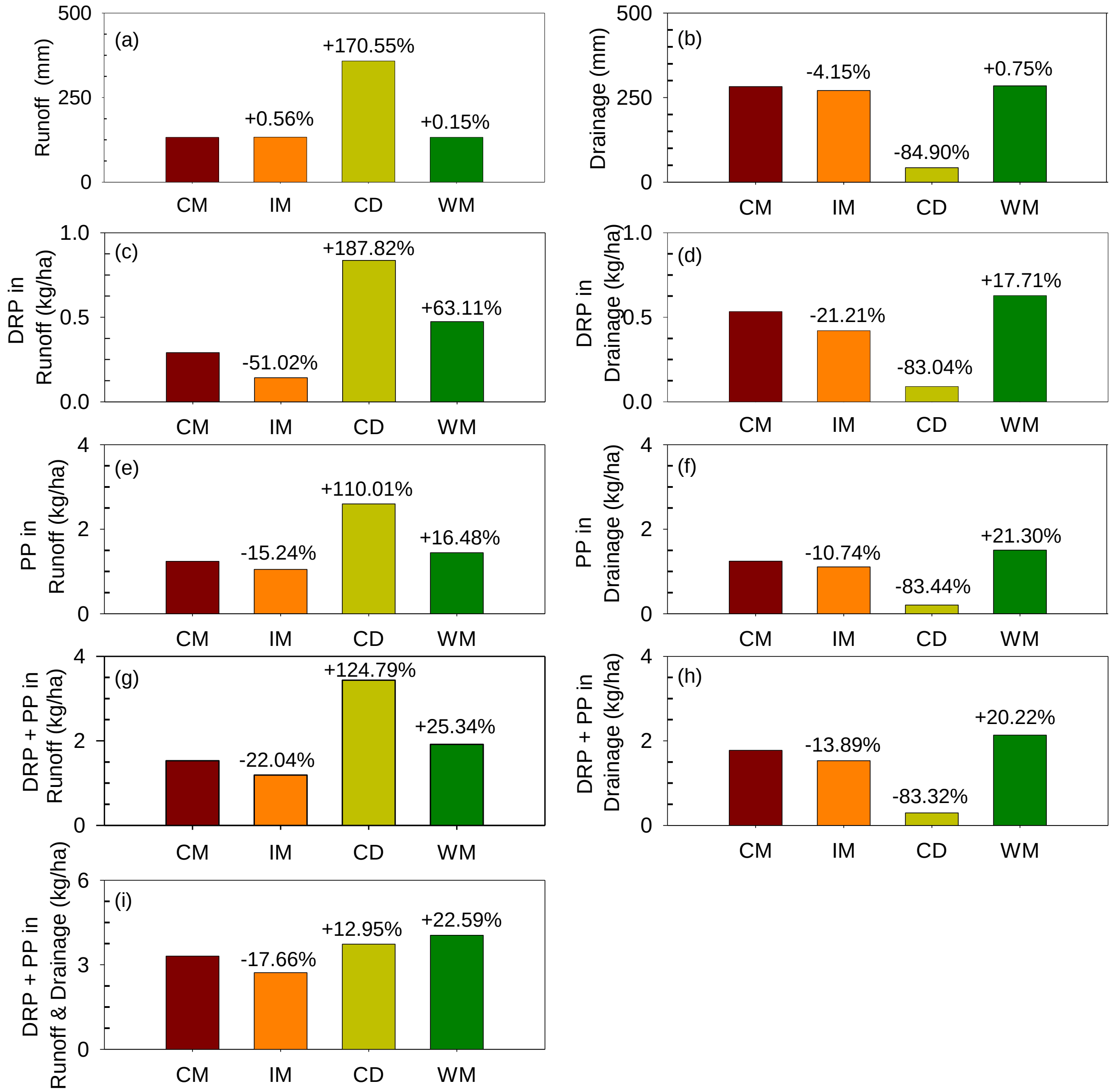

Figure 4.4: Comparison of RZWQM2-P simulation with conventional management practices (CM), injected manure application (IM), controlled drainage (CD) and winter manure application (WM) in terms of (a) Runoff, (b) Drainage, (c) DRP loss through surface runoff, (d) DRP loss through drainage, (e) PP loss through runoff, (f) PP loss through drainage, (g) DRP + PP loss through runoff, (h) DRP + PP loss through drainage, (i) DRP + PP loss through runoff + drainage. DRP, Dissolved Reactive Phosphorus; PP, Particulate Phosphorus.

Numbers on the top of each bars represents % increase (+)/decrease (-) over conventional management practices.

4.4 DISCUSSIONS

The RZWQM2-P model responded well in simulation of manure and soil P dynamics as suggested by P balance over the simulation period (Table 4.6). An inspection of simulated manure and soil P dynamics on randomly selected manure application year 2010-11 with maize planting shows that on the day of manure application P mass in P pools underwent an addition of 50 kg P /ha which reflected with increase in LabP pool (24 kg P ha^{-1}), ActIP pool (6 kg P ha^{-1}) and surface manure pool (20 kg P ha^{-1}). This sudden increase of LabP pool created an imbalance between LabP and ActIP pool of and about 18 kg P ha^{-1} absorbed into ActIP pool from LabP pool following the manure application. During the year 2010-11, 49 kg P ha^{-1}from LabP pool was taken up by the crop and on the day of harvest 30 kg P ha^{-1} was left as crop residue while the remaining 19 kg P ha^{-1} was grain harvested. This is comparable with the observed grain P harvested (17 kg P ha^{-1}) of maize at site under similar P application rate (Qi et al., 2017). During this year 27 kg P ha^{-1} of mineralized P is added to the system from plant residue and soil humus whereas total 5 kg P ha^{-1} was lost from system through surface runoff and tile drainage. Overall the simulated P for the whole simulation years is balanced (Table 4.3) out with annual average P input (25 kg P ha^{-1}from manure, 23 kg P ha^{-1}from plant residue and soil humus) is added up with annual average P output (43 kg P ha^{-1}of plant P uptake, 3 kg P ha^{-1}of P loss through transport pathways) and annual average change in soil P (increase of 2 kg P ha^{-1}).

The RZWQM2-P model is capable of simulating the partition of total P losses through different pathways in tile drained field with manure application. Several studies have shown that both surface runoff and tile drainage are important pathways for P loss from agricultural fields (Smith et al., 2015; Tan and Zhang, 2011; Zhang et al., 2015a). Simulation results showed that 54 % of total annual average total P loss (DRP + PP) was through tile flow, of which 75 % was PP (Table 4.6), and those values were 53% and 74%, respectively, based on observed data. P transfer from the soil to tile drainage water occurs through water movement through the soil matrix and/or preferential flow path. Preferential flow path was earlier identified as a principle mechanism for DRP and PP loss to tiles in the present study area (Tan et al., 2007; Tan and Zhang, 2011; Zhang et al., 2015 a, b). Simulation of RZWQM2-P model identified this fact satisfactorily with 82% of DRP whereas all of PP load to through tile drainage was transported by the macropore flow. In RZWQM2-P model, along with water flow volume, DRP loss through surface runoff and tile drainage greatly depend upon amount of LabP pool. Therefore, a satisfactory simulation of P dynamics will lead to reasonable estimation of LabP pool, which in turn effect the simulation of DRP loss through surface runoff and tile drainage. In a study, at the same site under similar management practices Wang et al., (2018b) reported that measured Olsen P in 0-150 mm of soil layer is within the range of 50-80 kg P ha^{-1} during the fall period. This value conforms to the RZWQM2-P simulated average LabP of 76 kg P ha^{-1} for the same depth of soil layer during the fall season. Along with acceptable simulation of P dynamics, the model's capability in simulation of P losses through tile flow is attributed to satisfactory soil moisture, soil matrix flux and macropore flux simulations. Adoptation of Richard's equation to simulate soil moisture and matrix flux whereas use of the Poiseuille's law based approach in simulation of macropore flow may resulted in satisfactory water flux through these flow pathways. The use of Hooghoudt's steady state equation may further facilitated tile drainage simulations which in turn impacted P losses through tile drainage. Soil temperature also plays an important role in simulating P dynamics while an acceptable soil temperature simulation may led to a good estimation of P flow rates among various P pools, decomposition and mineralization rates of residue and soil organic matter. Finally, the implementation of manure P pools as recommended by Vadas et al., (2007) may improved the simulation of dynamics and fate of applied manure P while considering leaching, physical assimilation and decomposition of manure P explicitly. Although RZWQM2-P satisfactorily simulated P losses (DRP, PP) through both surface runoff and tile drainage, further tests are recommended with more observed data in a tile drained agricultural field.

The management simulation suggested that controlled drainage would reduce total P loss (DRP +PP) through tile flow, but as it increased total P loss through surface runoff, overall it contributed towards 13 % more total P loss from the field considering both surface runoff and tile drainage than conventional management practices (Figure 4.4). Tan and Zhang (2011) found that total P loss was reduced through tile flow and it increased through surface runoff. But overall, controlled drainage reduced total P loss from the field considering both surface runoff and tile drainage, which conflicted with our study. This may be due to the fact that the greater amount of precipitation during our study period as compared to the same of Tan and Zhang (2011) (910 mm vs 781 mm) leads to more surface runoff (358mm vs 37 mm) consequently more P losses through surface runoff, which resulted in more overall total P losses from the field in our study. So, for the areas where frequent rainfalls lead to significant amount of surface runoff, controlled draiange is not a recommended management practice to reduce overall P losses from tile drained field. Winter manure application leads to more P losses (23% increase) as compare to conventional management practices. This is due to the fact that during the winter season majority of water outflow from the field occurs and winter manure application makes applied P vulnerable for loss under frequent runoff from snowmelt and rain on snow events. This simulation of winter manure application by RZWQM2-P agreed with the study of Liu et al., (2017a) who simulated the impact of fall and winter manure application on total P losses and found that this has increased annual total P losses loss by 12-16% over the spring application. Finally, simulation of injected manure application with RZWQM2-P indicated that instead of surface application, injected manure application into shallow soil profiles would decrease all forms of P losses from agricultural fields under similar agro-climatic conditions (Figure 4.4). This is attributed to the low availability of P on the soil surface for rain and runoff and better incorporation into soil profile due to injection of manure below the soil surface. These results concurred with the study of Daverede et al., (2004) who reported that injected manure application reduced DRP loading through surface runoff by 90% over the surface application.

Computer simulation models are built on assumptions and simplified version of the very complex real-world phenomenon so inevitably they have some limitations. In this context, RZWQM2-P model is limited to one dimension, field scale and treats soil as a homogeneous medium. The dissolved unreactive P loss is not being simulated under the present model science and so the P loss to groundwater. The model has limited capability in simulation of PP loss, as it assumes that particle bound P originates from the first 0.01 m soil layer and only the macropore flow contribute to tile drainage bound PP loss while bypassing the soil matrix. Another shortcoming of RZWQM2-P is that, being a field scale model, it cannot be applied over a large-scale watershed. At present, within RZWQM2-P the Richard's equation is solved iteratively, which slows down the simulation and calibration process of the model parameter based on the trial and error method. It utilizes a lot of resources. Therefore, for future improvement attention should be paid to adopting algorithms to accelerate the speed of solving the Richard's equation and auto calibration of model parameters.

4.5 CONCLUSIONS

In this study, the newly developed RZWQM2-P model, was assessed in simulating agricultural P losses in term of DRP and PP . The model assessment was done with eight years of data collected from a subsurface drained field with liquid cattle manure application and corn-soybean rotation in southwestern Ontario, Canada. The simulation results showed that the RZWQM2-P performed satisfactorily in simulating the DRP and PP losses both through surface runoff and subsurface drainage and were consistent with the observed trend that the non-growing season dominated the P losses over the growing season. The simulation resembles with the observed fact that tile drainage and surface runoff both equally contributed towards P losses and most P was lost as PP. The simulation suggested that preferential flow is the main pathway for P losses through tile drainage at the site. Furthermore the application of RZWQM2-P to quantify the impacts of three agricultural management practices indicated that the subsurface manure application rather than controlled drainage is an effective option to mitigate P losses from a tile drained cropland whereas winter manure application suggested increase in P losses from the field. Although, the developed RZWQM2-P appears to be a promising tool for P management in subsurface drained manured agricultural field, further tests are recommended with more observed data in a tile drained agricultural field.

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CONNECTING TEXT TO CHAPTER 5

Chapter 3 and Chapter 4 presented the development, evaluation, and applications of the newly developed RZWQM2-P model. The evaluation revealed satisfactory performance of the model's simulation of P losses both through surface runoff and tile drainage under inorganic fertilizer and manure application. The model simulation identified the injected manure application is a promising management strategy to reduce the P losses from an agricultural field. However, the RZWQM2-P model has many input parameters that governs P simulation thus making it time consuming to calibrate. So, a sensitivity analysis is employed to identify influential model parameters so that calibration process is only focused on them to simplify the modelling process. Chapter 5 presents a sensitivity analysis of the newly developed RZWQM2-P model to provide a guideline for its user in selection of the key parameters while calibrating the model.

The following manuscript based on the content of Chapter 5 has been prepared for publication in a peer reviewed international journal and it was co-authored by Zhiming Qi[1], Youjia Li[1], Tie-Quan Zhang[2], Chin S. Tan[2], and Liwang Ma[3].

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1. Department of Bioresource Engineering, McGill University, Sainte-Anne-de-Bellevue, Quebec, H9X 3V9, Canada

2. Harrow Research and Development Center, Agriculture and Agri-Food Canada, Harrow, Ontario, N0R 1G0, Canada

3. USDA-ARS Rangeland Resources and Systems Research Unit, Fort Collins, Colorado, 80526, USA.

CHAPTER 5

GLOBAL SENSITIVITY ANALYSIS OF RZWQM2-P IN SIMULATION OF AGRICULTURAL PHOSPHORUS LOSS

Debasis Sadhukhan[1], Zhiming Qi[1], Youjia Li[1], Tiequan Zhang[2], Chin S. Tan[2], Liwang Ma[3]

1. Department of Bioresource Engineering, McGill University, Sainte-Anne-de-Bellevue, Quebec, H9X 3V9, Canada

2. Harrow Research and Development Center, Agriculture and Agri-Food Canada, Harrow, Ontario, N0R 1G0, Canada

3. USDA-ARS Rangeland Resources and Systems Research Unit, Fort Collins, Colorado, 80526, USA.

ABSTRACT

In assessing how the output of a numerical model is influenced by its input parameters, sensitivity analysis provides a guideline in identifying and selecting key parameters while calibrating the model. Recently developed RZWQM2-P model, integrating a new phosphorus (P) module into the RZWQM2 model, was shown to successfully simulate P losses through surface runoff and tile drainage under different agricultural management practices. No global sensitivity analysis was performed for the newly developed RZWQM2-P model's simulation of P losses, leaving key parameters governing P losses simulation unidentified. The present study's objective was to address this shortcoming. Morris screening and Sobol-variance-based sensitivity analysis methods were applied to the prediction of dissolved reactive P (DRP) and particulate P (PP) losses through surface runoff and tile drainage. Data were collected from a liquid cattle manure applied experimental field with maize and soybean rotation in Ontario, Canada. Macroporosity proved to be a sensitive parameter in simulating P losses in all forms and from all outlets, while DRP loss

through surface runoff was most sensitive to the P extraction coefficient, and PP loss through surface runoff was mainly governed by Universal Soil Loss Equation (USLE) parameters. Tile flow DRP and PP losses were most sensitive to the plant P uptake distribution parameter and the soil detachability coefficient, respectively. These results will inform the development of guidelines for RZWQM2-P model calibration.

5.1 INTRODUCTION

Sensitivity analysis (SA) examines how variation in a numerical model's input parameters affects variation in the model's output. Depending upon whether the output variability is obtained by varying the input parameters across their entire feasible range or around a fixed reference value, SA is classified as global sensitivity analysis (GSA) or local sensitivity analysis (LSA), respectively (Norton et al., 2015). An LSA examines the one-at-a-time effect of a single input parameter on the model output while keeping other parameters at constant values. In contrast, GSA addressed variability in model output by considering simultaneous changes and resulting interactions among all input parameters over given ranges (Pianosi et al., 2016). However, GSA has high computation demands as it requires multiple model runs over a defined sample space (Pianosi et al., 2016; Norton et al., 2015; Vanuytrecht et al., 2014). Widely acknowledged in the literature as an essential and particularly well-suited tool for performing sensitivity analysis of environmental models (Saltelli et al., 2008; Pianosi et al., 2016), GSA procedures generally implements a screening method, followed by variance based methods (Pianosi et al., 2016; Saltelli et al., 2000; Vanuytrecht et al., 2014). The screening method is employed to reduce the computation cost of more robust variance-based methods (Pianosi et al., 2016).

Loss of P from an agricultural field through surface runoff and tile drainage is an extremely complex phenomenon involving soil physical, chemical, biological and hydrological processes occurring on and below the soil surface. The success of an agricultural P process control model greatly depends on how effectively and efficiently the model parameterizes these processes. Sadhukhan et al., (2019a) developed the RZWQM2-P model and satisfactorily calibrated and validated its simulation of dissolved reactive P (DRP) and particulate P (PP) losses through both surface runoff and tile drainage from a field amended with either inorganic P fertilizer and manure P application, and subject to a corn-soybean rotation (Sadhukhan et al., 2019 a, b). There being many input parameters governing P-loss processes, RZWQM2-P is difficult and time-consuming to calibrate. A sensitivity analysis (SA) could be applied to identify influential parameters, narrowing the focus of the calibration process to high impact parameters, thereby simplifying the modelling process. Accordingly, the present study was designed to perform GSA on the simulation of DRP and PP losses through surface runoff and tile drainage by the RZWQM2-P model. The study's specific objectives were to: (*i*) employ a Morris screening method (Morris, 1991) to screen and subsequently identify those P input parameters which have the greatest influence on model outputs, and (*ii*) employ Sobol's variance based method (Sobol, 1990) to quantify the most influential P parameters.

5.2 MATERIALS AND METHODS

5.2.1 RZWQM2-P Model

A P module enhanced extension of the USDA-ARS-developed RZWQM2 model (Ahuja et al., 2000), the RZWQM2-P model (Sadhukhan et al., 2019a) performs as a single model: the P module simulating P dynamics in an agricultural field, and RZWQM2 governing the physical, biological, chemical and hydrological processes that influence the P simulation — *i.e.*, crop growth, runoff, drainage, soil moisture and its flux, soil temperature, sediment yield, macropore flow, plant residue and soil humus decomposition and agriculture management practices such as controlled drainage and tillage. All these components are simulated by RZWQM2 within its original functionalities and then the P module uses them to simulate P dynamics and P losses through surface runoff and tile drainage. RZWQM2-P is a field scale, one dimensional agricultural process control model with a daily time step. The model employs the Richards equation (Richards, 1931) to simulate soil water redistribution within the soil profile following infiltration, the latter being simulated by the Green-Ampt method (Green and Ampt, 1911). Surface runoff is generated when the rainfall rate exceeds the infiltration rate and sediment yield is computed using USLE method (Wischmeier and Smith, 1978). Tile drainage flow is calculated by Hooghoudt's steady state equation (Bouwer and Schilfgaarde, 1963) and the macropore flow is governed by Poiseuille's law. Crop growth can be simulated by either embedded DSSAT 4.0 crop model (Jones et al., 2003) or a generic crop production model (Hanson, 2000), while evapotranspiration is estimated using the double layer Shuttleworth-Wallace model (Shuttleworth and Wallace, 1985). The P model within RZWQM2 model is designed as per Jones et al., (1984) and Vadas (2014). The RZWQM2-P model simulates DRP and PP loss through surface runoff using the methods developed by Neitsch et al., (2011) and McElroy et al., (1976), respectively, whereas it simulates tile drainage bound DRP and PP loss following Francesconi et al., (2016) and Jarvis et al., (1999), respectively.

5.2.2 Field Experiment & Input Data Collection

The data inputs required by the RZWQM2-P model include: (*i*) site specific information (latitude, longitude, elevation, area, slope etc.), (*ii*) soil physical and chemical properties, (*iii*) agricultural management practices data (crop planting, harvest, tillage, fertilization etc.), and (*iv*) daily meteorological data. An eight-year (June 2008 to April 2016) field study was conducted at the Hon. Eugene F. Whelan Research Farm near South Woodslee, ON (42.21N, 82.74W). The site housed 16 plots (67.1 m × 15.2 m) subject to different treatments, of which plots 4 and 14 received liquid cattle manure and were under free drainage (depth: 0.85 m, spacing: 3.80 m). The crop rotation followed an annual rotation of maize (*Zea mays* L.) and soybean [*Glycine max* (L.) Merr.]. Maize was planted in even years (2008, 2010, 2012 and 2014) at a density of 79,800 seeds ha^{-1}, while soybean was planted in odd years (2009, 2011, 2013, 2015) at a density of 486,700 seeds ha^{-1}. Prior to seeding, in corn years exclusively, liquid cattle manure an equivalent of 50 kg P ha^{-1} and 200 kg N ha^{-1} was surface-applied to the plots. Though manure water extractable P content was not formally measured, we assumed 60% of the liquid cattle manure's total P to be in that form (Kelinman et al., 2005). Chisel plow tillage occurred each year prior to planting and after harvest. Serving as RZWQM2-P soil input data, the properties of the clay loam soil of plots 4 and 14 were averaged across six soil horizons (Table 5.1). Prior to the onset of the experiment (2008), soil texture, field capacity (θ_{fc}), permanent wilting point (θ_{wp}), bulk density (ρ) and porosity (φ) were measured, along with soil labile P (as Olsen P - Olsen et al., 1954), and soil total P. Weather data (air temperature, precipitation, relative humidity, solar radiation and wind speed) to run the model were collected for the period of 1st Jan. 2008 to 31st Dec. 2016 by an automated meteorological weather station located at the Whelan farm, and located less than 500 m from the experimental plots. Sadhukhan et al., (2019b) used the same dataset to calibrate and validate the RZWQM2-P model. In the present study the calibrated soil hydraulic input parameters (Table 5.1) from that earlier study were adopted.

Table 5.1: Measured and calibrated soil physical and chemical properties at the study site

Soil Layer depth (mm)	Measured soil properties: ρ (kg m^{-3})	Clay (%)	Sand (%)	OM (%)	θ_{fc} (m^3 m^{-3})	φ (m^{-3} m^{-3})	θ_{wp} (m^{-3} m^{-3})	LabP (g kg^{-1})	TotalP (g kg^{-1})	Calibrated soil properties: P_b (cm)	λ	k_{sat} (cm h^{-1})	k_{lat} (cm h^{-1})
0-10	1330	34.2	29.0	3.7	0.37	0.54	0.18	0.02	0.90	-20.06	0.16	0.01	0.02
10-100	1330	34.2	29.0	3.7	0.37	0.54	0.18	0.02	0.90	-29.03	0.15	0.35	0.70
100-250	1390	34.2	29.0	3.7	0.36	0.54	0.18	0.02	0.90	-16.64	0.20	0.55	1.10
250-450	1390	40.7	25.7	2.0	0.35	0.50	0.18	0.01	0.65	-16.16	0.19	0.55	1.10
450-800	1330	40.4	27.0	0.7	0.36	0.48	0.18	0.01	0.50	-25.10	0.15	0.17	0.35
800-1200	1330	39.3	24.6	0.5	0.36	0.48	0.17	0.01	0.40	-35.17	0.14	0.17	0.35

ρ, Soil bulk density; OM, Soil organic matter content; θ_{fc}, Volumetric soil moisture content at field capacity; φ, Soil porosity; θ_{wp}, Volumetric soil moisture content at permanent wilting point; LabP, Soil labile P, TotalP, Soil total P; P_b, Air entry pressure; λ, Pore size index; k_{sat}, Saturated hydraulic conductivity; k_{lat}, Lateral hydraulic conductivity;

5.2.3 Sensitivity Analysis

5.2.3.1 Parameters

Based on experience gained during the manual calibration of RZWQM2-P to simulate DRP and PP losses through surface runoff and tile drainage for the same 8-year dataset (Sadhukhan et al., 2019b), parameters influencing P losses (Table 5.2) were selected to include in a GSA of the model. These parameters were assumed to be independent from one another and their probability density functions (PDF) to be uniformly distributed within a given range as the range of "input values usually has more influence on the output than the distribution shapes" (Haan et al., 1998).

Table 5.2: RZWQM2-P parameters selected for the sensitivity analysis and their ranges

Parameters	Symbol	Range
Macroporosity (m^3 m^{-3})	Mac	0.01 - 0.90
P extraction coefficient (-)	P_{exc}	0.10 - 1.00
Soil erodibility (t ha^{-1})	K	0.01 - 1.97
Cover and management factor	C	0.01 - 1.00
Support practice factor	P	0.01 - 1.00
Manning's N	N	0.01 - 0.40
Soil filtration coefficient (m^{-1})	K_f	0.01 - 1.00
Soil detachability coefficient (g J^{-1} mm^{-1})	K_d	0.01 - 1.00
Soil replenishment rate coefficient (gm m^{-2} day^{-1})	K_r	0.01 - 1.00
Plant P uptake distribution parameter	P_{up}	1.00 - 15.00

5.2.3.2 Morris Screening Method

Morris, (1991) established the powerful Elementary Effect Test (EET) (Saltelli et al., 2008), to screen parameters for inclusion in more detailed and time-consuming variance based SA (Ruano et al., 2012). As the Morris screening method ranks parameters according to their influence on the model's output within a reasonable number of model runs, the method is particularly suitable for models with many parameters and the need a great deal of computational resources. The method works by computing the mean (μ*) of *r* absolute finite differences, *i.e.*, the 'Elementary Effects (EE)' as (Campolongo and Saltelli, 1997):

$$\mu_i^* = \frac{1}{r}\sum_{j=1}^{r} |EE^j| = \frac{1}{r}\sum_{j=1}^{r} \left| \frac{Y\left(x_1^j, x_2^j, \dots x_i^j + \Delta_i^j \dots, x_M^j\right) - Y\left(x_1^j, x_2^j, \dots x_i^j \dots, x_M^j\right)}{\Delta_i^j} \right| \tag{5.1}$$

where,

i is the index of the parameters and $i = 1, 2, \cdots, M$

j is the index of the absolute finite differences and $j = 1, 2, \cdots, r$

r is the number of absolute finite differences for a given parameter,

x is the M-dimensional model input parameter vector, and $x = x_1, x_2, \cdots, x_M$

L is the number of levels (Pianosi et al., 2016), $L = 4$ in our study

M is the total number of input parameters subject to SA,

$Y(x)$ is the model output,

Δ_i is the input parameter variation, and $\Delta_i = \frac{L}{2 \cdot (L-1)}$

A parameter having a high μ* is deemed to be more influential, while a parameter with a high standard deviation (σ) of the EEs shows it to be interacting with other parameters as its sensitivity changes across the variability space.

5.2.3.3 Sobol's Variance-Based Method

Sobol's variance-based method (Sobol, 1990; Homma and Saltelli, 1996) takes a broader approach, quantifying parameter sensitivity as the proportion of the output variance due to the each parameter's individual effect compared to their overall combined effect. First-order sensitivity indices (S_i^F), or 'main effects (Eq. 5.2),' are computed in order to quantify the direct contribution of a parameter to the model's output variance, while total-order sensitivity indices (S_i^T) or the 'total effect,' (Eq. 5.3) measures the overall influence of an individual parameter considering it direct effect and its interaction with all the other parameters. The values of S_i^F and S_i^T vary from zero to one, with zero representing no sensitivity and one representing the highest possible sensitivity:

$$S_i^F = \frac{V[E_{x\sim i}(y|x_i)]}{V(y)} \tag{5.2}$$

$$S_i^T = \frac{E_{x\sim i}[V_{x_i}(y|x_{\sim i})]}{V(y)} \tag{5.3}$$

and

$$0 \leq S_i^F < S_i^T \leq 1 \tag{5.4}$$

where,

x~i	denotes all input parameters but the i^{th}
E	is the expected value,
V	is the variance.
i	is the index of the parameters and $i = 1, 2, \cdots, M$
M	is the total number of input parameters subject to SA,

5.2.3.4 Sample Generation and RZWQM2-P Simulation

The Morris screening method and the Sobol method required a tailored sampling technique. The required input samples for both methods were generated using the SAFE Toolbox (Sensitivity Analysis for Everybody, Pianosi et al., 2015) in Matlab (Mathworks, 2015) environment. For the Morris screening method, the Morris sampling strategy (Morris, 1991) was used with the values of $r = 100$ and $M = 10$ (Table 5.2), resulting in total number of model evaluations of $r(M+1) = 1{,}100$. For the Sobol's method, the top five most influential parameters were chosen as resulted from the Morris screening method. To generate the input sample for the Sobol's method, Pianosi et al., (2016) suggested all-at-a-time (AAT) sampling strategy was followed with a base sample size $N = 1{,}429$ and $M = 5$ resulted in $N(M+2) = 10{,}003$ model runs for each output. As the model had 4 outputs (DRP in runoff and tile and PP in runoff and tile), the total number of model evaluations was $10{,}003 \times 4 = 40{,}012$. The RZWQM2-P-simulated output was analyzed using Matlab (Mathworks, 2015) and sensitivity indices were computed with the help of the SAFE Toolbox (Pianosi et al., 2015).

The sensitivity analysis of RZWQM2-P required a considerable amount of time and computational resources. Under the present setup, a single run of the RZWQM2-P model using a PC with Intel® i7 dual core CPU operating at 3.60 GHz and using 8 GB RAM took about 3.5 minutes. Accordingly, to fully complete the Morris screening method it would take around 3 days while Sobol's method would take roughly 97 days to complete. To speed up the SA of RZWQM2-P, a computing parallelism technique was implemented. In our case, the parallelization and its preparation was automated by a Microsoft PowerShell® batch processing script. The script treated each logical core in the system as an individual computing unit, through multithreading technology that is accomplish by processor affinity assign. By using this methodology, the simulation of

RZWQM2-P was carried out parallelly in each logical core of an IBM BareMetal® windows server, Intel® Xeon Gold 5120 with 56 logical cores and 96 GB RAM. This take about 4 hrs. for Morris method and 7 days for Sobol's method to complete.

5.3 RESULTS

5.3.1 Morris screening method

The Morris method (Morris, 1991) allowed the screening of the RZWQM2-P model's parameter set (Table 5.2) while providing a qualitative ranking of the parameters for simulation of DRP and PP loss through surface runoff and tile drainage. Mean EEs (μ^*) of the parameters and their standard deviations (SD) (Figure 5.1) were considered the ranking criteria for the input parameters. The higher a parameter's μ^* value, the more influential that parameter; while the higher a parameter's SD the greater its degree of interaction with the other parameters. The ranking of top 5 most influential parameters for DRP and PP losses through surface runoff and tile drainage are presented in Table 5.3. The parameters P_{exc} and P_{up} were ranked highest in the simulation of DRP loss through surface runoff and tile drainage, respectively. For the PP loss through surface runoff, the USLE soil loss parameters (K, P, C) occupied the top ranked positions, whereas K_d was the top ranked parameter for PP loss through tile drainage. Macroporosity was ranked as an influential parameter in simulation of P losses particularly through tile drainage.

Table 5.3: Rank of P parameters based on Morris Screening Method in simulation of DRP in runoff, DRP in tile, PP in runoff and PP in tile.

Rank	DRP Runoff	DRP Tile	PP Runoff	PP Tile
1	P_{exc}	P_{up}	K	K_d
2	Mac	Mac	P	Mac
3	P_{up}	K_d	C	K_f
4	K_d	P_{exc}	Mac	K_r
5	K	K_f	K_f	P_{up}

DRP, Dissolved reactive phosphorus; PP, Particulate phosphorus; C: Cover and management factor; K: Soil erodibility; K_d: Soil detachability coefficient; K_f, Soil filtration coefficient; K_r, Soil replenishment rate coefficient; Mac, Macroporosity; P Support practice factor; P_{exc}, P extraction coefficient; P_{up}, Plant P uptake distribution parameter.

5.3.2 Sobol's variance based method

In the present study the Sobol's variance-based method (Sobol, 1990; Homma and Saltelli, 1996) was employed to compute the sensitivity of the top 5 most influential parameters (Table 5.3) in simulation of DRP and PP loss through surface runoff and tile drainage, as identified by the Morris screening method (Morris, 1991). The computed first order (S^F) and total order (S^T) sensitivity indices, for the parameters listed in Table 5.3, are presented in Figure 5.2. In simulation of DRP loss through surface runoff, P_{exc} and macroporosity individually contributed 51% and 27%, while overall they accounted for 73% and 42% respectively (Figure 5.2a). Simulation of DRP loss thorough tile drainage was mainly governed by P_{up} and macroporosity (Figure 5.2b), whereas P_{up} alone influenced 95% of the output variability and macroporosity overall influenced 47% of the output variability. Macroporosity was the main explanatory parameter in simulation of PP loss through surface runoff, contributing individually 42% of output variability, while the USLE soil loss parameters K, P, and C overall contributed 22%, 29% and 5%, respectively to simulating PP loss through surface runoff (Figure 5.2c). Simulation of PP loss through tile drainage was predominantly determined by K_d and macroporosity (Figure 5.2d) while other parameters like K_f, K_r and P_{up} overall contributed 55%, 43% and 38% of the output variability, respectively.

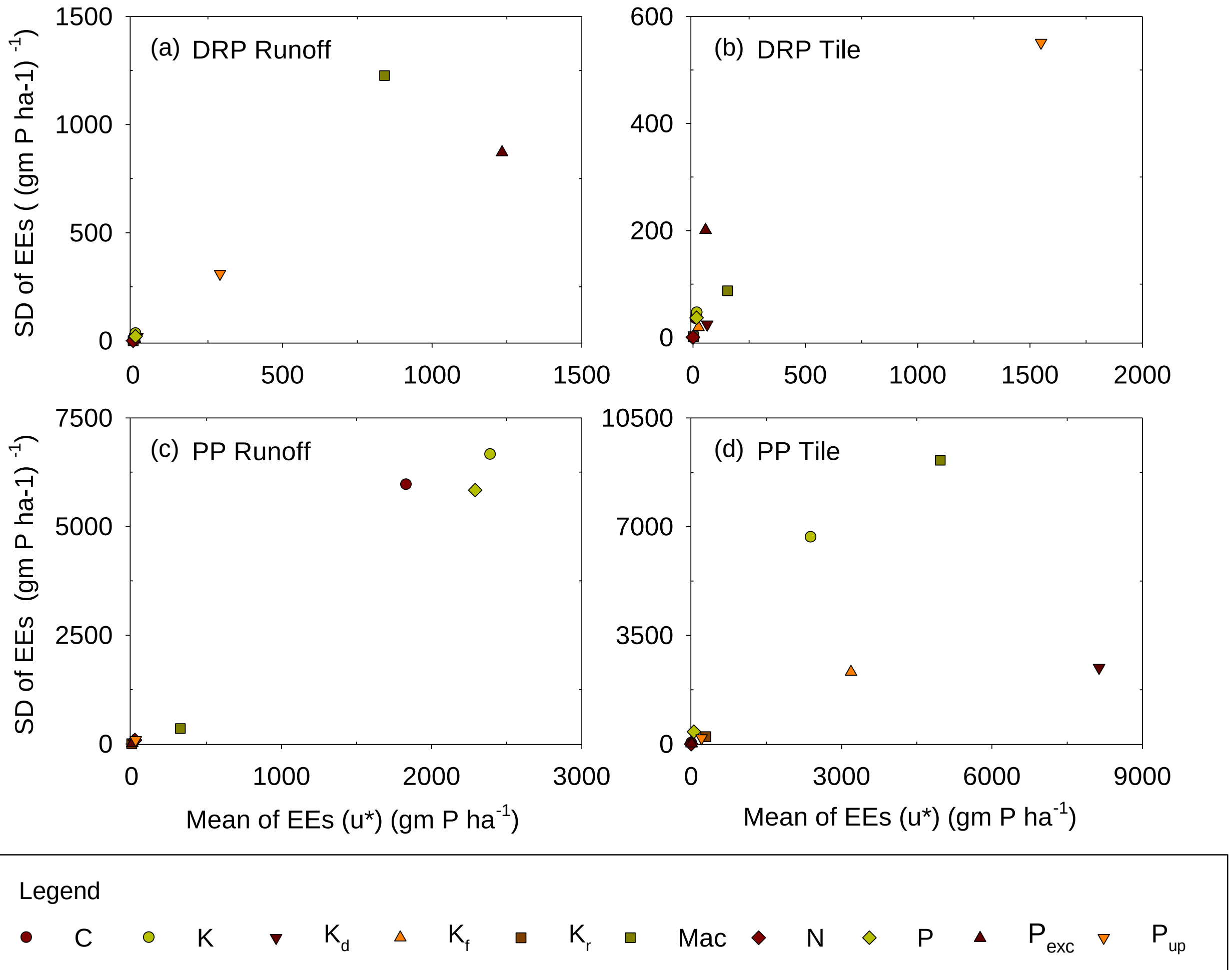

Figure 5.1: Mean EE and its SD for the RZWQM2-P's P parameters in simulation of a) DRP in runoff, b) DRP in tile, c) PP in runoff and d) PP in tile

EE: Elementary effect; SD: Standard deviation; DRP, Dissolved reactive phosphorus; PP, Particulate phosphorus; C: Cover and management factor; K: Soil erodibility; K_d: Soil detachability coefficient; K_f, Soil filtration coefficient; K_r, Soil replenishment rate coefficient;

Mac, Macroporosity; N, Manning's N, P Support practice factor; P_{exc}, P extraction coefficient; P_{up}, Plant P uptake distribution parameter.

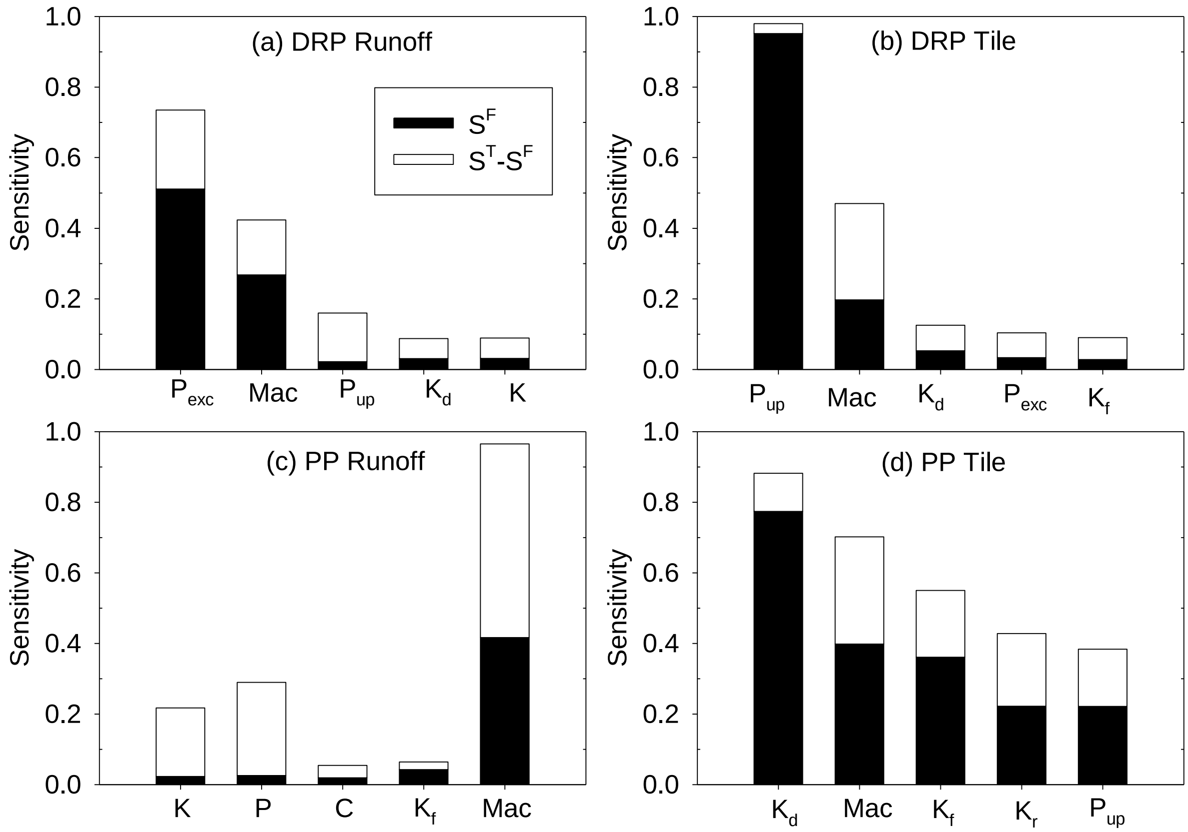

Figure 5.2: 1st order (S^F) and Total sensitivity (S^T) indices in simulation of a) DRP in runoff b) DRP in tile c) PP in runoff and d) PP in tile.

DRP, Dissolved reactive phosphorus; PP, Particulate phosphorus; C: Cover and management factor; K: Soil erodibility; K_d: Soil detachability coefficient; K_f, Soil filtration coefficient; K_r, Soil replenishment rate coefficient; Mac, Macroporosity; P Support practice factor; P_{exc}, P extraction coefficient; P_{up}, Plant P uptake distribution parameter.

5.4 DISCUSSION

Sensitivity analysis showed that P loss outputs of the RZWQM2-P model were influenced by several input parameters; however, certain input parameters (e.g., macroporosity) had a dominant role in the simulation of P losses (Figure 5.2). This substantiates earlier findings that the preferential flow path is the principle mechanism for DRP and PP loss in the present study area (Sadhukhan et al., 2019a; Tan et al., 2007; Tan and Zhang, 2011; Zhang et al., 2015a, 2015b). Macroporosity is a measurable parameter, so while calibrating this model, care should be taken to determine its value reliably. As demonstrated by the calculated sensitivity coefficients (Figure 5.2b & 2c), P_{up} had a significant influence on DRP loss simulation through tile drainage whereas K_d, K_f and K_r had their greatest impact on simulated PP loss through a tile drainage system. This occurred because a plant's P uptake from the soil labile P pool through its root system (represented by P_{up}) limits the availability of labile P in the soil profile which would otherwise be lost as DRP through the tile drainage system. Whereas K_d controls the detachment of soil particles to which P is attached, K_f controls filtration as they pass through the soil profile and K_r governs their replenishment. While P_{up} , K_d, K_f and K_r are time consuming and costly to measure in field experiments, so a user of the RZWQM2-P model should prudently choose the value of these parameters while calibrating the model.

The value of P_{exc} was found to be highly correlated (Figure 5.2a) with the RZWQM2-P's simulation of the DRP loss through surface runoff. This signifies that DRP in surface runoff is mainly influenced by the size of the labile P pools in topmost soil layer. Accordingly, while calibrating the model, care should be taken in determining the size of the labile P pool of the topmost soil layer. The simulation of PP loss through surface runoff is sensitive to the USLE soil loss coefficients (K, P, C) (Figure 5.2c), which control the yield of sediment to which P is attached.

Accordingly, attention must be paid to these parameters when calibrating PP loss through surface runoff.

A systematic sensitivity analysis requires a certain amount of information about the model's input parameters, such as parameter distributions and minimum/maximum values, *i.e*., the range of values within which the input parameters vary. In the present case, we were able to find parameter ranges from the literature, but very little information was available regarding parameter distributions. We made the seemingly arbitrary assumption that all parameters were distributed uniformly over their given range; however, the parameter distribution assumptions have been found to not significantly affect the outcome on sensitivity analyses (Haan and Zhang, 1996; Fontaine et al., 1992). Another restriction in the present study was the limited available computational resources as under the present setup. In our case, a single RZWQM2-P scenario took about 3.5 minutes to complete. Given the total of roughly 50 input parameters (including hydraulic and crop parameters) needed for the simulation of P losses in the RZWQM2-P model, a gigantic and cumbersome number of model runs would be necessary to perform sensitivity analysis. Therefore, a choice of the ten number of input parameters (Table 5.2) that would be subjected to the sensitivity analysis was made based on previous experience (Sadhukhan et al., 2019 a, b) in manually calibrating the model. At present, within RZWQM2-P, the Richard's equation is solved iteratively, which slows down the simulation process and uses a considerable amount of resources. Additionally, the exclusivity of RZWQM2-P on a Microsoft Windows® operating system restricts us to fully utilizing available high-performance computational resources. Therefore, for future improvement, attention should be paid to adopting algorithms to accelerate the speed of solving the Richard's equation and to develop a LINUX version of the model.

5.5 CONCLUSIONS

In this study, a global sensitivity analysis was performed following a Morris screening method and a Sobol's variance-based method for the RZWQM2-P model in simulation of DRP and PP loss through surface runoff and tile drainage. RZWQM2-P's P loss simulations depended upon many parameters, however, macroporosity was the preeminent parameter in simulation of all form of P losses. Others parameters that substantially impacted P loss simulation were P_{up} (98% for tile DRP) , K_d (85% for PP tile) K_f (45% for PP tile), K_r (40% for PP tile) , P_{exc} (75% for DRP runoff) and USLE soil loss coefficients (>10% for PP runoff). The key model parameters identified in this study will provide a guideline during the future calibration process of the model.

ACKNOWLEDGMENTS

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CHAPTER 6

GENERAL SUMMARY AND CONCLUSION

6.1 GENERAL SUMMARY

Phosphorus (P) is becoming a scarce resource day by day as its demand is ever increasing particularly for agricultural sector. P being a crucial nutrient for maintaining plant growth and crop yield, is mainly added to the agricultural fields in the form of fertilizer and/or manure. Due to uncontrolled and non-scientific fertilizer / manure application, this applied P is being lost along with the water outflow (surface runoff, tile drainage) from the agricultural field and is finally being ended at the freshwater bodies (River, Lakes), causing widespread algal bloom leading to water quality degradation. Latest, research in this regard, had identified that agricultural fields those having tile drainage system in it, is contributing most towards this P loss. To manage the P loss from agricultural fields, we need to understand the hydrological, physical and bio-chemical processes which are involved in crop P uptake, P movement within the soil profile and soil water, and transportation of P through runoff, tile drainage and sediments. Researchers had recommended that computer simulation models could be efficiently employed to accomplish this task. However, as of present day there seems a lack of P simulation computer models particularly to simulate P loss from tile drained agricultural field. Hence, this research has been undertaken and the overall goal of this research was to develop a computer simulation model to simulate P loss through different hydrological pathways from an agricultural field and embedded it into RZWQM2 model. The P model was designed with five different soil P pools (Jones et al., 1984) with dedicated P pools for to simulate P dynamics due to the manure and fertilizer applications (Vadas, 2014). The developed P model has advance capabilities to simulate tile bound DRP (Francesconi et al., 2016) and PP losses (Jarvis et al., 1991; Larsson et al., 2007). Subsequently, developing the model and integrating it with the RZWQM2 model, its evaluations have been done twice, once with the manure application and another time with fertilizer application. A global sensitivity analysis of the RZWQM2-P was also performed to identify the most influential model parameter in relation to P loss simulation.

6.2 CONCLUSIONS

Objective 1: To develop a computer simulation model to simulate P loss through different hydrological pathways from an agricultural field, based on the most recent scientific findings regarding the fate and transport of P.

A new P model is developed while assigning the soil P in five different soil P pools: three inorganics, namely labile P (LabP), active inorganic P (ActIP) and stable inorganic P (StabIP) and two organic pools namely fresh organic P pool (FrsOP) and stable organic P pool (StabOP) respectively, following the nomenclature of Jones et al., (1984). Besides these soil P pools, as an advanced feature, the P model has four surface manure P pools and two surface fertilizer P pools to simulate P dynamics arising from the application of fertilizer and manure (Vadas et al., 2004, 2007, 2008; Vadas, 2014). The manure P pools are inorganic water extractable P(ManWIP), inorganic stable P (ManSIP), organic water extractable P (ManWOP), and organic stable P (ManSOP). The fertilizer P pools are available fertilizer P (AvFertP) and residual fertilizer P (ResFertP) pool. These independent manure and fertilizer P pools enable the model to simulate more precisely the P dynamics arising from the application of fertilizer and manure in an agricultural field. Among these P pools, plant can uptake P for its growth from the LabP pool only and it is considered to be in plant available dissolved form. Applied P in the form of manure/fertilizer is distributed within the manure P pools / fertilizer P pools based on application depth, type and properties of manure/fertilizer applied. For the liquid manure/fertilizer application, it is assumed that 60% of the applied P immediately infiltrates into the soil added to the soil P pools (LabP, ActP) of the topmost soil layer (Vadas et al., 2007). Leached and/or decomposed P from the manure/fertilizer P pools are incorporated to the soil P pools (LabP, ActP). The absorption and desorption of P among the inorganic soil P pools is simulated based on Jones et al., (1984) with advanced dynamic absorption and desorption rate as prescribed by Vadas et al., (2006). This latest modification enables the model to simulate P movement among these pools by using a dynamically changing rate factor rather than a constant rate factor. Mineralization and immobilization of P is simulated based on Jones et al., (1984). The P model simulates tile drainage bound DRP and PP loss following Francesconi et al., (2016) and Jarvis et al., (1999) respectively. The model assumes that particle bound P originates from the first soil layer of the soil profile and PP through soil profile is only transported through the macropore flow and contributes directly to the tile system bypassing the soil matrix. In the model DRP and PP loss through surface runoff is simulated as per Neitsch et al., (2011) and McElroy et al., (1976) respectively. LabP and two manure water extractable P pools contribute to DRP loss whereas all the P pools contribute to PP loss.

Objective 2: To incorporate the developed P model into the RZWQM2 model.

The newly developed P model described above successfully incorporated into the RZWQM2 model. While the P model simulates P dynamics, the RZWQM2 governs the physical, biological, chemical, and hydrological processes that influence the P simulation. The developed P model combined with RZWQM2 is known as RZWQM2-P which performs as a single tool. The P model being dependent on RZWQM2 for the simulation of crop growth, runoff, drainage, soil moisture and its flux, soil temperature, sediment yield, macropore flow and agriculture management practices. All these components are simulated by RZWQM2 within its original functionalities and then the P model uses model outputs to simulate P dynamics and P losses (DRP, PP) through surface runoff and tile drainage from an agricultural field.

Objective 3: To test, calibrate and validate the newly developed RZWQM2-P model in North American condition.

The newly developed RZWQM2-P model was successfully evaluated twice to test its capability in simulation of DRP and PP loss through surface runoff and tile drainage from agricultural field using the observed P loss and water flow data collected from a subsurface-drained corn-soybean rotated field with clay loam soil in southwestern Ontario, Canada. The first evaluation corresponded to test the model's response of fertilizer application while the second was for the manure application. The simulation results of both the tests showed that the RZWQM2-P model performed satisfactorily in simulating the DRP and PP losses through both surface runoff and subsurface tile drainage and were consistent with the observed trend that the non-growing season dominated the P losses over the growing season. The simulation resembled with the observed fact that most P was lost as PP and tile drainage contributed majority of P loss. The simulation also suggested that preferential flow is the main pathway for P losses through tile drainage at the site. The RZWQM2-P model's acceptable P loss simulating ability particularly through tile drainage can be attributed to the adoption of the Richards's equation for simulation of soil matrix flow, and the Hooghoudt's equation for simulation of tile drainage flow. The use of Poiseuille's law may have resulted in better macropore flow simulations, which led to better simulations of PP loading to the tile system. The newly developed P module integrated with RZWQM2 is a promising tool for agricultural P management, particularly for subsurface-drained fields.

Objective 4: To perform a sensitivity analysis of the developed RZWQM2-P model in order to identify the most sensitive parameters of the model in relation to P simulation.

A global sensitivity analysis was performed following a Morris screening method and a Sobol's variance-based method for the RZWQM2-P model in simulation of DRP and PP loss through surface runoff and tile drainage. To perform the sensitivity analysis data were collected from a liquid cattle manure applied experimental field with maize and soybean rotation in Ontario, Canada. The sensitivity analysis identified RZWQM2-P's P loss simulations depended upon many parameters, however, macroporosity was the preeminent parameter in simulation of all form of P losses. The DRP loss through surface runoff was most sensitive to the P extraction coefficient, and PP loss through surface runoff was mainly governed by Universal Soil Loss Equation (USLE) parameters. Tile flow DRP and PP losses were most sensitive to the plant P uptake distribution parameter and the soil detachability coefficient. The key model parameters identified in this study will provide a guideline during the future calibration process of the model.

6.3 CONTRIBUTIONS TO KNOWLEDGE

The research performed as presented in this thesis led to several contributions to knowledge as follows,

1. A new P simulation model for the tile drained agricultural field is successfully developed, which many researchers earlier identified as an urgent need to understand P dynamics in an agricultural field.
2. The RZWQM2 model has now became more versatile as an agricultural process control model with added P simulation capability.
3. The developed RZWQM2-P model has a potential to serve as a valuable tool for agricultural planners and environmental stakeholders to evaluate different agricultural

management practices suitable to reduce P loading from agricultural field to the surface water bodies.

4. This study is an example of how a process-based model can be developed and applied to model P losses from agricultural fields. The study can also be used as a valuable guide and reference for future modelling studies.

6.4 RECOMMENDATIONS FOR FUTURE RESEARCH

1. Newly developed RZWM2-P model needs to be further tested at several other locations under different soil, climate, and crop rotations for a longer period with more observed data.

2. The RZWQM2-P needs to be applied to evaluate the impact of control drainage, control drainage with sub-irrigation and different tillage methods on P losses from agricultural fields.

3. The RZWQM2-P model is a field scale, one dimensional model and treats soil as a homogeneous medium. Further research can be carried out to upgrade it to the watershed scale, multidimensional model and that treats soil as a heterogeneous medium.

5. At present, within RZWQM2-P, the Richard's equation is solved iteratively, which not only slows down the simulation process but also consumes a considerable amount of time and computational resources. So, in future research it is recommended to modify the model code to adopt algorithms to accelerate the speed of solving the Richard's equation.

6. The exclusivity of RZWQM2-P on a Microsoft Windows® operating system restricted us to fully utilizing available high-performance computational resources. Therefore, the future research can be directed towards the development of a LINUX version of the model.

APPENDIX-A

RZWQM2-P GOVERNING EQUATIONS

A1 INITIALIZATION OF P POOLS

Before the start of model simulations, the soil P pools need to be initialized. Initial amount of labile P pool, stable organic P pool and fresh organic P pool are needed to be specified by the model user. Other P pools are initialized as follows.

Active P Pool is initialized as:

$$ActP = Labp * \frac{1-PSP}{PSP} \tag{1}$$

Where, ActP = Active P amount in a soil layer (kg/ha)

Labp = Labile P amount in a soil layer (kg/ha)

PSP = Phosphorus sorption coefficient (or P availability index) (Williams et al., 2008)

PSP is calculated as follows

$$PSP = -0.045 * Log(Clay) + 0.001 * LabP - 0.035 * SoilOC + 0.43 \tag{2}$$

Where, Clay = Clay % of soil

Labp = Labile P amount in a soil layer (mg/kg)

SoilOC = Soil Organic Carbon (%)

$$SoilOC = SoilOM * 0.58 \tag{3}$$

Where, SoilOM = Soil organic matter in a layer (%)

Inorganic Stable P pool is initialized as:

$$StabiP = 4 * ActP \quad (4)$$

Where, StabiP = Stable Inorganic P pool in a soil layer. (kg/ha)

ActP = Active P amount in a soil layer (kg/ha)

All the surface manure and fertilizer P pool are initialized as zero.

A2 FERTILIZER P DYNAMICS

Model assumes that when a fertilizer is applied the fertilizer P is instantaneously is divided between two surface fertilizer pools based on depth of application namely available fertilizer P pool and residual fertilizer P pool. 75% of fertilizer P is added to available fertilizer pool and 25% is added to residual fertilizer pool (Vadas, 2014; Williams, 1969). The P in the available fertilizer pool is readily available to be lost by runoff and to be adsorbed by soil. The adsorbed fertilizer P is added to the soil labile P pool of the first soil layer.

So, in case of surface applied fertilizer i.e. depth of application is zero

$$AvfertP = 0.75 * FertP \quad (5)$$

$$ResfertP = 0.25 * FertP \quad (6)$$

And in case of subsurface application

$$AvfertP = 0.75 * Fertp * Fsurf \quad (7)$$

$$ResfertP = 0.25 * Fertp * Fsurf \quad (8)$$

Where, Avfertp = Available fertilizer P pool (kg)

Resfertp = Residual fertilizer P Pool (kg)

FertP = Fertilizer P applied in the field (kg)

Fsurf = Fraction of fertilizer left on surface during application (-)

The fraction of FertP which is applied below soil surface is directly added to the soil labile P pool depending upon a factor based on the ratio of soil layer thickness to fertilizer application depth.

For a layer having depth less than fertilizer application depth

$$Fact = \frac{Tsoil}{FertD} \tag{9}$$

For the soil layer where the fertilizer is applied

$$Fact = 1 - \sum_{1}^{k} Fact_k \tag{10}$$

$$LabP_a = LabP_b + FertP * Fact * (1 - Fsurf) \tag{11}$$

Where, Fact = A factor (-)

Tsoil = Thickness of a soil layer (m)

FertD = Fertilizer application depth (m)

$LabP_b$= Labile P pool of a soil layer before subsurface fertilizer application. (kg)

$LabP_a$= Labile P pool of a soil layer after subsurface fertilizer application. (kg)

k = Number of soil layers having depth less than fertilizer application depth. (-)

After the fertilizer application, once the rainfall happens all the P in Avfertp pool is released. For the second rainfall, 40% of the P in Resfertp is released and from the third rainfall onwards, consistently about 7.5% of the remaining P in Resfertp was released until all the P in Resfertp pool is exhausted (Vadas et al., 2008).

So, for the case of first rainfall event

$$Fertprelease = AvfertP \tag{12}$$

For the case of 2nd rainfall event

$$Fertprelease = 0.40 * ResfertP \tag{13}$$

For the case of 3rd rainfall onwards

$$Fertprelease = 0.075 * ResfertP \tag{14}$$

Where, Fertprelease = Amount of P is released due to rainfall from the fertilizer P pools. (kg)

This released P is either lost through runoff or absorbed in soil labile P pool with infiltration or both depending upon a factor based on rainfall and runoff (Vadas, 2014; Vadas et al., 2008). Factor, that represents the distribution of released fertilizer P between runoff and infiltration and is calculated as

$$PDFACTOR = 0.034 * e^{(3.4 * \frac{Runoff}{Rainfall})} \tag{15}$$

Where, PDFACTOR = P distribution factor

Runoff = Runoff amount (cm)

Rainfall = Rainfall amount (cm)

So, P concentration in runoff water due to loss of P from fertilizer P pool

$$FertPcrunoff = \frac{Fertprelease * PDFACTOR}{Rainfall * Area * 100} \tag{16}$$

Where, FertPcrunoff = P concentration in runoff water due to loss of P from fertilizer P pool (kg/m^3)

Area = Area of the field (ha)

P mass in in runoff water due to loss of P from fertilizer P pool is calculated as

$$FertPmrunoff = FertPcrunoff * Runoff * Area * 100 \tag{17}$$

Where, FertPmrunoff = P mass in in runoff water due to loss of P from fertilizer P pool (kg)

The amount of P mass that is released but not carried away by runoff is adsorbed to the soil labile pool as follows

$$LabP_a(1) = LabP_b(1) + (Fertprelease - Fertpmrunoff) * 0.8 \quad (18)$$

$$LabP_a(2) = LabP_b(2) + (Fertprelease - Fertpmrunoff) * 0.2 \quad (19)$$

Where, $LabP_a$ (1) = Labile P pool of first soil layer after adsorption. (kg)

$LabP_b$ (1) = Labile P pool of first soil layer before adsorption. (kg)

$LabP_a$ (2) = Labile P pool of second soil layer after adsorption. (kg)

$LabP_b$ (2) = Labile P pool of second soil layer before adsorption. (kg)

In between, the first rainfall event and fertilizer application, the P in the Avfertp is being absorbed in the soil and added to soil labile P pool of the first soil layer. But this absorption rate varies according to the land cover type. It does at a slower rate for grassed or residue-covered soils than for bare soils (Vadas et al., 2008; Williams, 1969). The equations used to calculate the fraction of applied fertilizer P that remains available on the soil surface over time after application are

For bare soil:

$$Fertpfr = -0.16 * \ln(Days) + 0.65 \quad (20)$$

For reside covered soil:

$$Fertpfr = -0.16 * \ln(Days) + 0.75 \quad (21)$$

From crop covered soil:

$$Fertpfr = -0.16 * \ln(Days) + 0.85 \quad (22)$$

Where, Fertpfr = Fraction of P in AvFert pool remaining after absorption. (-)

Days = Number of days since application. (Days)

A3 MANURE P DYNAMICS

To simulates manure P dynamics user need to specify the day of manure application , the % percentage of manure left on surface during application (100% for surface application, 0% for total sub-surface application), mass of manure applied, manure dry matter content (%), P content (kg/ha) (%), water extractable inorganic P content (%), water extractable organic P content (%). At the day of manure application, the applied manure P is divided into four surface manure P pools based on P content, water extractable inorganic P content, water extractable organic P content, type of application i.e. weather surface or subsurface, and type of manure i.e. weather liquid or solid. In case of liquid manure i.e. the manure with dry mater content less than 15%, model assumes that 60% of manure P immediately infiltrates into soil and added the respective soil active and labile P pools (Vadas et al., 2004, 2006). At the time of manure application, the manure P is distributed in four surface manure P pools namely manure water extractable inorganic P pool, manure water extractable organic P pool, manure stable inorganic P pool, manure stable organic P pool. Water extractable P pools represent P that can be released from manure by rain and stable P pools represents P that can be released by rain but can be transformed to water extractable pools as manure decomposes and mineralizes (Vadas et al., 2007) . The size of the water extractable inorganic and organic P pool are determined based on the percentage of water extractable inorganic P and percentage of water extractable organic P present in the manure. The difference between manure total P and sum of water extractable inorganic P and water extractable organic P is the stable P. The model divides this stable P into inorganic and organic P pools according to 25/75 ratio (Ajiboye et al., 2004; Dou, et al., 2000; He, et al., 2003; He and Honeycutt, 2001; He et al., 2006; McDowell and Stewart, 2005; McGrath et al., 2005; Turner et al., 2004; Vadas, 2014).

$$Manwip = (Manpmass * S * L) * \frac{Manweipper}{100} \tag{23}$$

$$Manwop = (Manpmass * S * L) * \frac{Manweopper}{100} \tag{24}$$

$$Mansop = (Manpmass * S * L) * (1 - \frac{Manweipper}{100} - \frac{Manweipper}{100})*0.75 \tag{25}$$

$$Mansip = (Manpmass * S * L) * \left(1 - \frac{Manweipper}{100} - \frac{Manweipper}{100}\right) * 0.25 \tag{26}$$

Where, Manwip = Manure water extractable inorganic P Pool. (kg)

Manwop = Manure water extractable organic P Pool. (kg)

Mansip = Manure stable inorganic P pool. (kg)

Mansop = Manure stable organic P pool. (kg)

Manpmass = Manure P mass applied. (kg)

Manweipper = Percentage of water extractable inorganic P (%)

Manweopper = Percentage of water extractable organic P (%)

S =fraction of manure P mass left on surface during application (1 for surface application, 0-1 for subsurface application.

L = Fraction of manure P mass stay on surface after infiltration of manure P into the soil during application (0.4 for liquid manure, 1 for solid manure)

In case of liquid manure, the 60% manure P is absorbed to the soil active and labile P pool as follows

$$ActP_a(1) = ActP_b(1) + (Manpmass * S * (1 - L)) * \left(1 - \frac{Manweipper}{100} - \frac{Manweipper}{100}\right) * 0.25 \tag{27}$$

$$\begin{aligned} LabP_a(1) = {} & LabP_b(1) + \left(Manpmass * S * (1 - L)\right) * \frac{Manweipper}{100} \\ & + \left(Manpmass * S * (1 - L)\right) * \frac{Manweopper}{100} * 0.95 \\ & + \left(Manpmass * S * (1 - L)\right) * \left(1 - \frac{Manweipper}{100} - \frac{Manweipper}{100}\right) * 0.75 * 0.95 \end{aligned} \tag{28}$$

$$LabP_a(2) = LabP_b(2) + \left(Manpmass * S * (1 - L)\right) * \frac{Manweopper}{100} * 0.05$$

$$+ \left(Manpmass * S * (1 - L)\right) * \left(1 - \frac{Manweipper}{100} - \frac{Manweipper}{100}\right) * 0.75 * 0.05 \qquad (29)$$

Where, $LabP_a$ (1) = Labile P pool of first soil layer after absorption. (kg)

$LabP_b$ (1) = Labile P pool of first soil layer before absorption. (kg)

$LabP_a$ (2) = Labile P pool of second soil layer after absorption. (kg)

$LabP_b$ (2) = Labile P pool of second soil layer before absorption. (kg)

$ActP_a$ (1) = Active P pool of first soil layer after absorption. (kg)

$ActP_b$ (1) = Active P pool of first soil layer before absorption. (kg)

In case of sub-surface application of manure, the manure P which is applied below ground surface is directly added to soil labile P and active P pool depending upon a factor based on the ratio of soil layer thickness to manure application depth as follows.

For a layer having depth less than manure application depth

$$Fact = \frac{Tsoil}{ManD} \qquad (30)$$

For the soil layer where the manure is applied

$$Fact = 1 - \sum_1^k Fact_k \qquad (31)$$

$$LabP_a = LabP_b + \left(Manpmass * (1 - S)\right) * \frac{Manweipper}{100} * Fact$$

$$+ \left(Manpmass * (1 - S)\right) * \frac{Manweopper}{100} * Fact$$

$$+ (Manpmass * (1 - S)) * \left(1 - \frac{Manweipper}{100} - \frac{Manweipper}{100}\right) * 0.75 * Fact \qquad (32)$$

$$ActP_a = ActP_b + (Manpmass * (1 - S)) * \left(1 - \frac{Manweipper}{100} - \frac{Manweipper}{100}\right) * 0.25 * Fact \qquad (33)$$

Where, Fact = A factor (-)

Tsoil = Thickness of a soil layer (m)

ManD = Manure application depth (m)

$LabP_b$= Labile P pool of a soil layer before subsurface manure application. (kg)

$LabP_a$= Labile P pool of a soil layer after subsurface manure application. (kg)

$ActP_a$= Active P pool of a soil layer after subsurface manure application. (kg)

$ActP_b$= Active P pool of a soil layer before subsurface manure application. (kg)

k = Number of soil layers having depth less than manure application depth. (-)

After manure application, as the manure ages, manure and P in the Mansip, Mansop, Manwop Pool decomposes and assimilates based on ambient temperature and manure moisture content (Vadas, 2014).

Daily manure decomposition rate is calculated as

$$\mathrm{Mandcomr} = 0.003 * TFA^{0.5} \tag{34}$$

Where, Mandcomr = Manure decomposition rate (per day)

TFA = Unit less temperature factor (-). Varies between 0-1.

TFA depends on daily atmospheric temperature and it is calculated as

$$TFA = \frac{2*32^2*T^2-T^4}{32^4} \tag{35}$$

Where, T = Average daily atmospheric temperature (^{0}C)

Daily manure assimilation rate is calculated as

$$Manasimr = 30.0 * e^{(2.5*Moist)} \tag{36}$$

Where, Manasimr = Manure assimilation rate (per day)

Moist = Unit less Manure moisture content factor (-). Varies between 0-0.9

Moist depends on amount of rainfall and it is calculated as

If no rainfall i.e. rainfall amount = 0

$$Moist = Moist_0 - \left(0.075 - 0.05 * \frac{ManMass}{Appiled\ ManMass}\right) * TFA \tag{37}$$

If rainfall is less than 4 mm

$$Moist = Moist_0 \tag{38}$$

If rainfall is more than 4 mm

$$Moist = Moist_0 + (0.27 - 0.3 * Moist_0) \tag{39}$$

Where, $Moist_0$ = Manure moisture factor of the previous day. (-)

TFA = Temperature factor. (-)

ManMass = Current manure mass present in the field. (kg)

Applied ManMass = Initial amount of manure applied in the field. (kg)

Manure decomposition is calculated as

$$Mandcom = \text{ManMass} * \text{Mandcomr} \tag{40}$$

Where, Mandcom = Manure decomposition. (kg/day)

Manure coverage area also decomposes at a same ratio as manure decomposes

$$Mancovadcom = \frac{Mandcom}{Manmass} * Mancov \tag{41}$$

Where, Mancovadcom = Manure cover area decomposition (ha/day)

Mancov = Manure Cover area (ha)

Decompositions of P from Mansop, Mansip, Manwop Pool is calculated as

$$Mansopdcom = 0.01 * Mansop * MIN(TFA, Moist) \tag{42}$$

$$Mansipdcom = 0.0025 * Mansip * MIN(TFA, Moist) \tag{43}$$

$$Manwopdcom = 0.1 * Manwop * MIN(TFA, Moist) \tag{44}$$

Where, Mansopdcom = Manure stable organic P decomposition. (kg/day).

Mansipdcom = Manure stable inorganic P decomposition. (kg/day).

Manwopdcom = Manure water extractable organic P decomposition. (kg/day).

Mansop = Manure stable organic P pool. (kg)

Mansip = Manure stable inorganic P pool. (kg)

Manwop = Manure water extractable P pool. (kg)

75% of the decomposed P from Mansop is added to Manwip pool and remaining 25% is added to Manwop pool. All the decomposed Mansip and Manwop pool is added to Manwip pool (McGrath et al., 2005).

Manure assimilation is calculated as

$$Manasim = Manasimr * TFA * Mancov \tag{45}$$

Manure cover area and Manure P pools are assimilated at the same ratio as the manure mass assimilate as follows

$$Mancovasim = \frac{Manasim}{Manmass} * Mancov \tag{46}$$

$$Manwipasim = \frac{Manasim}{Manmass} * Manwip \tag{47}$$

$$Manwopasim = \frac{Manasim}{Manmass} * Manwop \tag{48}$$

$$Mansipasim = \frac{Manasim}{Manmass} * Mansip \tag{49}$$

$$Mansopasim = \frac{Manasim}{Manmass} * Mansop \tag{50}$$

Where, Mancovasim = Manure cover area assimilation. (ha/day)

Manwipasim = Manwip pool assimilation (kg/day)

Manwopasim = Manwop pool assimilation (kg/day)

Mansipasim = Mansop pool assimilation (kg/day)

Mansopasim = Mansip pool assimilation (kg/day)

Assimilated P is added to the soils labile and active P pools. 60% of assimilated P is added to the respective P pool of the first soil layer. If the depth of the 2[nd] layer is less than 15 cm then 30% of it is added to the respective P Pools 2nd soil layer and rest 10% is added the respective P pools of to the 3rd soil layer. If the depth of the 2nd layer is more than 15 cm then 40% of assimilated P is added to the respective P pool of the 2nd soil layer (Vadas, 2014).

$$ActP_a(1) = ActP_b(1) + Mansipasim * 0.6 \tag{51}$$

$$LabP_a(1) = LabP_b(1) + (Manwipasim + Manwopasim + Msopasim) * 0.6 \tag{52}$$

If the depth of the second layer is more than 15 cm then

$$ActP_a(2) = ActP_b(2) + Mansipasim * 0.4 \tag{53}$$

$$LabP_a(2) = LabP_b(2) + (Manwipasim + Manwopasim + Msopasim) * 0.3 \tag{54}$$

If the depth of the second layer is less than 15 cm then

$$ActP_a(2) = ActP_b(2) + Mansipasim * 0.3 \tag{55}$$

$$ActP_a(3) = ActP_b(3) + Mansipasim * 0.1 \tag{56}$$

$$LabP_a(2) = LabP_b(2) + (Manwipasim + Manwopasim + Msopasim) * 0.3 \tag{57}$$

$$LabP_a(3) = LabP_b(3) + (Manwipasim + Manwopasim + Msopasim) * 0.1 \tag{58}$$

After daily manure assimilation and decompositions the Manure mass, Manure coverage area and manure P pools are updated as follows

$$Manmass_a = Manmass_b - Mandcom - Manasim \tag{59}$$

$$Mancov_a = Mancov_b - Mancovdcom - Mancovasim \tag{60}$$

$$Mansip_a = Mansip_b - Mansipdcom - Mansipasim \tag{61}$$

$$Mansop_a = Mansop_b - Mansopdcom - Mansopasim \tag{62}$$

$$Manwop_a = Manwop_b - Manwopdcom - Manwopasim + Mansopdcom * 0.25 \tag{63}$$

$$Manwip_a = Manwip_b - Manwipasim + Manwopdcom + Mansopdcom * 0.75 + Mansipdcom \tag{64}$$

a,b stand for manure mass , coverage are and pool sizes after and before a particular day respectively.

When rainfall occurs, P from manure water extractable pools is released. This released P is either carried away by runoff or absorbed in soil labile P pool of the first soil layer. The amount of P release depends on rainfall amount and rain to manure mass ratio (Vadas et al., 2005; Vadas et al., 2004). Amount of P release from manure water extractable pools is released is calculated as

$$\text{Manprelease} = \text{Manextrc} * (\text{Manwip} + \text{Manwop}) \tag{65}$$

Where, Manprelease = Manure P release due to rainfall (kg /day)

Manextrc = Manure extraction coefficient (Per day). It value varies between 0-1

If no rainfall then Manextrc = 0.

Manextrc is calculated as

For dairy and beef manure

$$Manextrc = \frac{1.2 * W}{W + 73.1} \tag{66}$$

For Poultry and swine manure

$$Manextrc = \frac{2.2 * W}{W + 300.1} \tag{67}$$

Where, W is rain to manure mass ratio (cm^3/gm) and is calculated as

$$W = \frac{Rain}{Manmass} * Mancov * 10^5 \quad (68)$$

Where, Rain = Amount of rainfall. (cm)

$Manmass$ = Manure mass. (kg)

Mancov = Manure coverage area. (ha)

If runoff happens, then this released P from manure water extractable P pools are carried away by runoff, the concentration of released P in runoff water depends upon phosphorus distribution factor (PDFACTOR) and it is calculated (Vadas et al., 2005) as

$$\text{PDFACTOR} = (\frac{Runoff}{Rain})^{0.225} \quad (69)$$

Where, Runoff = Runoff amount. (cm)

Rain = Rainfall amount. (cm)

Manure P concentration in runoff water is calculated as

$$\text{Manpcrunoff} = \frac{Manprelease}{Rain*Area*100} * PDFACTOR \quad (70)$$

Where, Manpcrunoff = Manure P concertation in runoff. (kg/m^3)

Manure P mass loss through runoff is calculated as

$$Manpmrunoff = Manpconrunoff * Runoff * Area * 100 \quad (71)$$

Where, Manpmrunoff = Manure P mass loss through runoff. (kg)

Area = Area of field. (ha)

The manure P which is released from manure water extractable P pools but not carried through runoff is absorbed to soil labile p pools. 60% of it is added to labile p pool of the first soil layer.

In case of the depth of 2nd soil layer is more than 15cm then remaining 40% is added to the labile P pools of 2nd soil layer. If the depth of 2nd soil layer is less than 15cm then 30% of it added to labile pool of the 2nd soil layer and 10% is added to soil labile pool of 3rd soil layer.

$$Lab_a(1) = Lab_b(1) + (Manprelease - Manpmassrunoff) * 0.6 \tag{72}$$

If the depth of the second soil layer is more than 15 cm

$$Lab_a(2) = Lab_b(2) + (Manprelease - Manpmassrunoff) * 0.4 \tag{73}$$

If the depth of the second soil layer is less than 15 cm

$$Lab_a(2) = Lab_b(2) + (Manprelease - Manpmassrunoff) * 0.3 \tag{74}$$

$$Lab_a(3) = Lab_b(3) + (Manprelease - Manpmassrunoff) * 0.1 \tag{75}$$

A4 SOIL P DYNAMICS

There are constant sorption and desorption of P among the soil inorganic P pools (Figure 3.1) in order to maintain an equilibrium among the inorganic P pools. A rapid sorption and desorption exists between labile and active p pool, this is simulated based on Jones et al., (1984), with advance dynamic absorption and desorption (Vadas et al., 2006). The absorption and desorption of P between labile P and active P pool is depends upon P sorption coefficient (PSP) (Williams et al., 2008) and it is calculated as

$$PSP = -0.045 * Log(Clay) + 0.001 * LabP - 0.035 * SoilOC + 0.43 \tag{76}$$

An equilibrium is maintained between labile P and active P pool until the PBAL as defined by f equation 77 is zero. When PBAL >0, P from labile P pool moved to active P pool and when PBAL <0, P from active P pool moves to labile p pool.

$$PBAL = LabP - ActP * \frac{PSP}{1-PSP} \tag{77}$$

The movement of P from labile P pool to active P pool is calculated as i.e. when PBAL > 0

$$PFlow_{lab \to Act} = P_{srpf} * PBAL \tag{78}$$

The movement of P from active P pool to labile P pool is calculated as i.e. when PBAL < 0

$$PFlow_{act \to lab} = P_{dsrpf} * |PBAL| \tag{79}$$

Where, PBAL = A variable as defined by equation no 77. (kg/ha)

$Pflow_{lab->act}$ = P flow from labile P pool to active P pool. (kg/ha)

$Pflow_{act->lab}$= P flow from active P pool to labile P pool (kg/ha)

P_{srpf} = P sorption factor (-)

P_{dsrpf} = P desorption factor (-)

P_{srpf} and P_{dsrpf} dynamically changes daily as follows

$$P_{srpf} = A * Day^{B} \tag{80}$$

$$A = 0.918 * e^{-4.603*PSP} \tag{81}$$

$$B = -0.238 * Ln(A) - 1.126 \tag{82}$$

Where, A = A factor as calculated by equation no 81

B = A factor as calculated by equation no 82

Day = Cumulative day since when the P in labile p pool increased and created an imbalance with active P pool and P movement from labile P pool to active p pool starts.

$$P_{dsrpf} = Base * Day^{-0.29} \tag{83}$$

$$Base = -1..08 * PSP + 0.79 \tag{84}$$

Where, Base = A factor as defined by equation 84.

Day = Cumulative day since when P in active P pool increased and created an imbalance with labile p pool and P movement from active P pool to labile P pool starts.

Similarly a slow absorption and desorption happens between P in active P pool and stable inorganic P pool. An equilibrium between active P pool and stable inorganic P pool is maintained as long as PBAL1 as defined by equation 85 is zero. When PBAL1>0, P from active P pools moved to stable inorganic P pool and when PBAL1<0, P from stable inorganic P pool pools moved to active P pool.

$$PBAL1 = 4 * ActP - StabiP \tag{85}$$

P flow from active P pools moved to stable inorganic P pool i.e. when PBAL1>0 is calculated as

$$Pflow_{actp \to stabip} = 0.0006 * PBAL1 \tag{86}$$

P flow from stable inorganic P pool pools moved to active P i.e. when PBAL1<0 is calculated as

$$Pflow_{stabip \to actp} = 0.00006 * |PBAL1| \tag{87}$$

Where, $Pflow_{actp\text{->}Stabip}$ = P flow from active P to stable inorganic P pool. (kg/ha)

$Pflow_{stabip\text{->}actP}$ = P flow from stable inorganic P pool to active P pool. (kg/ha)

PBAL1 = A variable as defined by equation 86. (kg/ha)

Mineralization happens from fresh organic P pool and 80% of this mineralized P is added to soil labile P pool and remaining 20% is added to stable organic P pool (Jones et al., 1984). Mineralization is calculated as

$$Frsopmin = Frsominr * Frsop \tag{88}$$

Where, Frsopmin = Fresh organic P mineralization (kg/ha/day)

Frsopminr = Fresh organic P mineralization rate (per day)

Frsop = Fresh organic P Pool. (kg/ha)

$$Frsopminr = K_{or} * \sqrt{\gamma_{temp}\gamma_{water}} * \gamma_{ntr}$$

$$K_{or} = 0.8 \quad when\ \frac{Crpres}{Crpres_i} > 0.8$$
$$= \ 0.05\ \ when\ 0.1 < \frac{Crpres}{Crpres_i} < 0.8$$
$$= \ 0.0095\ when\ \frac{Crpres}{Crpres_i} < 0.1 \qquad (89)$$

Where, K_{or} = Rate constant (per day)

Mineralization also happens from stable organic P pool, and all the mineralized P from stable organic P pool is added to the labile P pool (Jones et al., 1984). Mineralization from stable organic P pool is calculated as

$$Stabopmin = K_{os} * MIN\left(\gamma_{temp} * \gamma_{water}\right) * Stabop \qquad (90)$$

Where, Stabopmin = Mineralization from stable organic P pool. (kg/ha/day)

K_{os} = rate constant of stable organic P mineralization =0.0003 per day

Stabop = P in stable organic P pool. (kg/ha)

Immobilization happens from labile P pool. The immobilized P from labile P pool is added to soil fresh organic P pool (Jones et al., 1984). Immobilization from labile P pool is calculated as

$$Labpimmo = 0.16 * R_{or} * \frac{P_m}{O_m} \qquad (91)$$

Where Labpimmo = Immobilization from labile P pool to fresh organic P pool. (kg/ha/day)

P_m/O_m = It depends on Labile P amount and it varies between 0.01 and 0.02.

$$\frac{P_m}{O_m} = 0.02 \; if \; LabP > 10$$

$$= 0.01 + 0.001 * Labp \qquad if \; LabP < 10 \tag{92}$$

R_{or} = Immobilization rate (per day)

$$R_{or} = K_{or} * Crpres * \sqrt{\gamma_{temp} * \gamma_{water}} * \gamma_{ntr} \tag{93}$$

A5 PLANT P UPTAKE

Plant need P for its growth. The governing equations of plant P uptake were adopted from Neitsch et al., (2011) and they are as follows. Fraction of P in the plant biomass on a given day in case of optimal plant growth is calculated as

$$f_{rp} = \left(f_{rp1} - f_{rp3}\right)\left[1 - \frac{f_{rphu}}{f_{rphu} + \exp\left(P_1 - P_2 \cdot f_{rphu}\right)}\right] + f_{rp3} \tag{94}$$

Where, f_{rp} = Fraction of P in plant biomass on a given day, in case of optimal plant growth

f_{rp1} = Normal fraction of P in plant biomass at emergence.

f_{rp3} = Normal fraction of P in plant biomass at maturity.

f_{rphu} = Fraction of potential heat unit (PHU) accumulated for the plant on a given day.

P_1, P_2 are shape coefficients. These are calculated as follows

$$P_1 = ln\left[\frac{f_{rphu,50\%}}{1 - \frac{f_{rp2} - f_{rp3}}{f_{rp1} - f_{rp3}}} - f_{rphu,50\%}\right] + P_2 \cdot f_{rphu,50\%} \tag{95}$$

$$P_2 = \frac{ln\left[\frac{f_{rphu,50\%}}{1-\frac{f_{rp2}-f_{rp3}}{f_{rp1}-f_{rp3}}}-f_{rphu,50\%}\right]-ln\left[\frac{f_{rphu,100\%}}{1-\frac{f_{rp\sim3}-f_{rp3}}{f_{rp1}-f_{rp3}}}-f_{rphu,100\%}\right]}{f_{rphu,100\%}-f_{rphu,50\%}} \tag{96}$$

Where, f_{rp2} = Normal fraction of P in plant biomass at 50% maturity.

$f_{rp\sim3}$= Normal fraction of P in plant biomass at near maturity.

$f_{rphu, 50\%}$ = Fraction of potential heat unit (PHU) accumulated for the plant at 50% maturity. = 0.5

$f_{rphu, 100\%}$ = Fraction of potential heat unit (PHU) accumulated for the plant at 100% maturity. = 1

Model assumes the value of ($f_{rp\sim3}$ - f_{rp3}) = 0.0001, in order to avoid the second ln term in the equation 96 to become undermined.

Optimal mass of P that should be stored in plant biomass on a given day is calculated as

$$Bio_{p,opt} = f_{rp} * Bio \tag{97}$$

Where, $Bio_{p, opt}$ = Optimum mass of P that should be stored in plant biomass on a given day. (kg/ha)

Bio = Total plant biomass of a given day. (kg/ha)

Plant P demand for a day is calculated as

$$P_{demand} = 1.5 * MIN(\, Bio_{p,opt} - Bio_p, 4 \cdot f_{rp3} \cdot \Delta\text{Bio}) \tag{98}$$

Where, P_{demand} = Plant P demand on a given day. (kg/ha)

Bio_p = Actual Plant P in a given day. (kg/ha)

ΔBio = Potential increase in total plant biomass on a given day. (kg/ha)

The P_{up} amount of P is up taken by the plant from the soil labile P pool only. The depth distribution of plant P uptake is calculated as

$$P_{up,z} = \frac{P_{demand}}{1-\exp\left(-\beta_p\right)}\left[1 - \exp\left(-\beta_p \frac{z}{z_{root}}\right)\right] \tag{99}$$

Where, $P_{up,z}$ = Potential P uptake from the soil surface to depth z (kg/ha)

β_p = Plant P uptake distribution parameter.

z = Depth from soil surface. (m)

z_{root} = Depth of root in soil from the soil surface on a given day. (m)

The potential P uptake from a soil layer is calculated by

$$P_{up,ly} = P_{up,zl} - P_{up,zu} \tag{100}$$

Where, $P_{up,\,ly}$ = Potential P uptake from a soil layer. (kg/ha)

$P_{up,\,zl}$ = Potential P uptake from soil surface to the lower boundary of the soil layer. (kg/ha)

$P_{up,\,zu}$ = Potential P uptake from soil surface to the upper boundary of the soil layer. (kg/ha)

Finally, the actual P uptake by the plant from a soil layer is calculated as

$$P_{act,ly} = MIN(P_{up,ly}, P_{demand}\,, LabP_{ly}) \tag{101}$$

Where, $P_{act,\,ly}$ = Actual P uptake by the plant from a layer. (kg/ha)

P_{demand} = P uptake demand not met by the overlaying soil layers. (kg/ha)

$LabP_{ly}$ = P in labile P pool of the layer. (kg/ha)

If the all the P demand of the crop can't not be met by soil labile P pool then, the plant under goes P stress and the yield get reduced. P stress is calculated as

$$P_{stress} = 1 - \frac{\varphi_p}{\varphi_p + \exp\,(3.535 - 0.02597\varphi_p)} \tag{102}$$

Where, P_{stress} = P stress for a given day.

φ_p = Scaling factor for P stress and it is calculated as

$$\varphi_p = 200 \cdot \left[\frac{Bio_p}{Bio_{p,opt}} - 0.05\right] \tag{103}$$

A6 P FLOW FROM RESIDUE AND SOIL ORGANIC MATTER

To simulate the P flow from the crop residue and soil organic matter the crop residues and soil organic matter are divided into five computational P pools as described within the soil nutrient module of the RZWQM2 model (Ma et al., 2012). The crop residue is divided into two pools namely fast residue pool and slow residue pool whereas Soil organic matter is divided into three pools namely fast organic matter pool, intermediate organic matter pool and slow organic matter pool. At beginning of the simulation P mass in these pools are initialized using the user defined initial C: P ratio. The P in these pools are decomposed daily at the same rate of carbon decomposition as computed (Rojas and Hanson, 2000) by the RZWQM2 model P is transferred within pools as shown in Figure A.2. P released due to degradation of residue pools will be added to the Fresh Organic P pool and P released due to the degradation of soil organic matter pools is added to stable organic P pool.

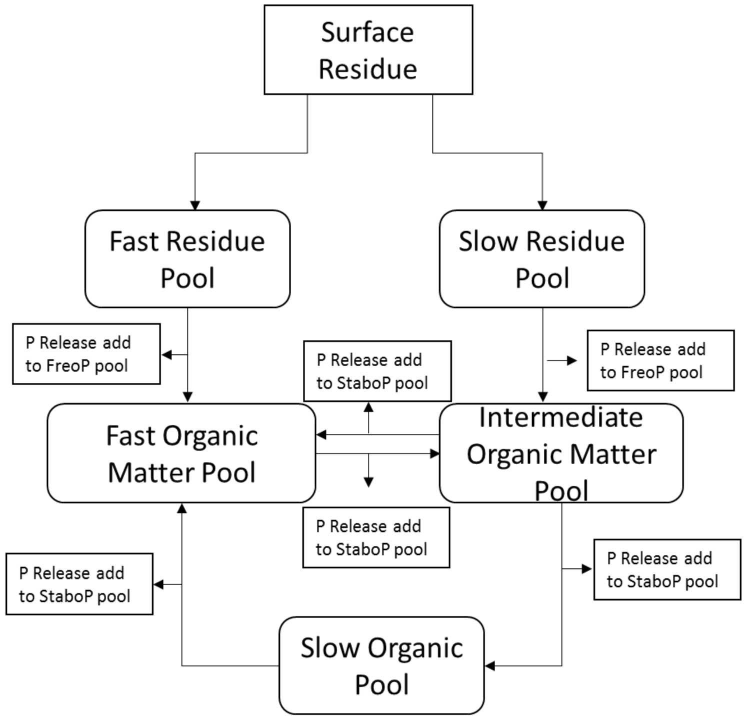

Figure A.2: P low from Residue and Soil Organic mater

A7 TILLAGE

Tillage operation incorporates the surface P pools i.e. fertilizer P pools and manure P pools into soil based on tillage incorporation efficiency and mixes the soil P pools and crop residues based on tillage mixing efficiency, tillage depth and ratio of soil mass of a layer to total soil mass of layers up to tillage depth. During tillage operation fertilizer P pools and manure water extractable P pools incorporates into soil labile P pool whereas the manure stable P pools incorporates into the active P pool of the first soil layer.

$$LabP_a(1) = LabP_b(1) + (Avfertp + Resfertp + Manwip + Manwop) * \frac{Tillinceffi}{100} \quad (104)$$

$$ActP_a(1) = ActP_a(1) + (Mansip + Mansop) * \frac{Tinceffi}{100} \quad (105)$$

Where, $LabP_a$ (1) = Labile P of the first soil layer after the incorporation due to tillage. (kg)

$LabP_b$ (1) = Labile P of the first soil layer before the incorporation due to tillage. (kg)

$ActP_a$ (1) = Active P of the first soil layer after the incorporation due to tillage. (kg)

$ActP_b$ (1) = Active P of the first soil layer before the incorporation due to tillage. (kg)

Tinceffi = Tillage incorporation efficiency. (%)

Tillage operation also mixes the soil P pools and crop residues of all the layers having depth less than tillage depth as follows

$$LabP_a = \left(1 - \frac{Tmixeffi}{100}\right) LabP_b + TlabP * Soil_{ratio} * \frac{Tmixeffi}{100} \quad (106)$$

$$ActP_a = \left(1 - \frac{Tmixeffi}{100}\right) ActP_b + TActP * Soil_{ratio} * \frac{Tmixeffi}{100} \quad (107)$$

$$StabiP_a = \left(1 - \frac{Tmixeffi}{100}\right) StabiP_b + TStabiP * Soil_{ratio} * \frac{Tmixeffi}{100} \quad (108)$$

$$StaboP_a = \left(1 - \frac{Tmixeffi}{100}\right) StaboP_b + TStaboP * Soil_{ratio} * \frac{Tmixeffi}{100} \quad (109)$$

$$FrsoP_a = \left(1 - \frac{Tmixeffi}{100}\right) FrsoP_b + TFrsoP * Soil_{ratio} * \frac{Tmixeffi}{100} \quad (110)$$

Where, $LabP_a$ = Labile P pool after the mixing due to tillage. (kg)

$LabP_b$ = Labile P pool before the mixing due to tillage. (kg)

$ActP_a$ = Active P pool after the mixing due to tillage. (kg)

$ActP_b$ = Active P pool before the mixing due to tillage. (kg)

$StabiP_a$ = Stabip P pool after the mixing due to tillage. (kg)

$StabiP_b$ = Stabip P pool before the mixing due to tillage. (kg)

$StaboP_a$ = Stabop P pool after the mixing due to tillage. (kg)

$StaboP_b$ = Stabop P pool before the mixing due to tillage. (kg)

$FrsoP_a$ = Frsop P pool after the mixing due to tillage. (kg)

$FrsoP_b$ = Frsop P pool before the mixing due to tillage. (kg)

TLabP = Sum of the P of all the soil labile P pool for the layers having depth less than tillage depth. (kg)

TActp = Sum of the P of all the soil active P pool for the layers having depth less than tillage depth. (kg)

TStabiP =Sum of the P of all the soil Stabip P pool for the layers having depth less than tillage depth. (kg)

TStabop = Sum of the P of all the soil Stabop P pool for the layers having depth less than tillage depth. (kg)

TFrsoP = Sum of the P of all the soil Stabop P pool for the layers having depth less than tillage depth. (kg)

$Soil_{ratio}$ = The ratio of soil mass of a layer to the total soil mass of the layers having depth less than tillage depth. (kg)

Tmixeffi = Tillage mixing efficiency. (%)

A8 DRP LOSS RUNOFF

Dissolve reactive P (DRP) loss through runoff is calculated as

$$Drplossrnf = Fertpmrunoff + Manpmrunoff + Labpmrunoff \tag{111}$$

Where, Drplossrnf = Amount of DRP loss through runoff. (kg/ha)

Fertpmrunoff = Fertilizer P loss through runoff. (kg/ha) [Section A2]

Manpmrunoff = Manure P loss through runoff. (kg/ha) [Section A3]

Labpmrunoff = Soil labile P loss through runoff. (kg/ha)

Labpmrunoff is calculated following Neitsch et al., (2011) as

$$Labpmrunoff = \frac{Pextr * LabP(1) * Runoff}{\rho_{b1} * Dsoil(1) * K_{d1}} \tag{112}$$

Where, Pextr = P extraction coefficient

Labp (1) = P in labile P pool of the first soil layer. (kg/ha)

Runoff = Amount of surface runoff on a given day. (m)

ρ_{b1} = Bulk density of the first soil layer. (kg/m3)

Dsoil (1) = Depth of the first soil layer. (m)

K_{d1} = Soil partitioning coefficient of the first soil layer (m3/kg)

Soil partitioning coefficient is depend on fraction of clay content of soil and is calculated as

$$K_{d1} = 0.1 + 0.25\ clay(1) \tag{113}$$

Where, clay (1) = Fraction of clay content of the first soil layer. (-)

A9 PP LOSS RUNOFF

Particulate Phosphorus (PP) loss through surface runoff is calculated based on Neitsch et al., (2011) as

$$PPlossrnf = 0.001 * Conc_{sedp} * \frac{sed}{Area} * Encr \tag{114}$$

Where, PPlossrnf = Amount of PP loss through runoff (kg/ha)

$Conc_{sedp}$ = Concentration of P attached to sediment in the surface soil layer. (gm P/MT soil)

Sed = Sediment yield on a given day. (MT)

Area = Area of the field. (ha)

Encr = P enrichment ratio (-)

$$Conc_{sedp} = 100 \frac{LabP(1) + ActP(1) + Stabip(1) + Stabop(1) + Frsop(1) + Avfertp + Resferp + Manwip + Manwop + Mansop + Mansip}{\rho_{b1} * Dsoil(1)} \tag{115}$$

$$Encr = 0.78 * Conc_{sed,rnf}^{-0.2468} \tag{116}$$

Where,

Encr = P enrichment ratio (-)

$Conc_{sed,\ rnf}$ = Concentration of sediment in runoff (Mg/m^3)

$$Conc_{sed,rnf} = \frac{sed}{10*Area*runoff} \tag{117}$$

Where, Sed = Sediment yield on a given day. (MT)

Area = Area of the field. (ha)

Runoff= Amount of surface runoff on a given day. (mm)

A10 DRP LOSS TILE DRAINAGE

To simulate DRP loss through tile drainage linear groundwater reservoir based approach as suggested by TAM-MO-DEL (Steenhuis et al., 1997) is used. In this approach DRP through matrix flow and as well as macropore flow at first contributes to the groundwater reservoir, from which then DRP is lost along with the drainage water.

Amount of P leached out from a layer by matrix flow is calculated as (Francesconi et al., 2016)

$$P_{Leach,mat} = C_{labp,SW}\left(1 - \exp\left(\frac{-q_{mat}}{K_d m_s + SW}\right)\right) \tag{118}$$

Where, $P_{leach, mat}$ = Amount of DRP loss through matrix flow from a soil layer. (kg/m^3)

$C_{labp, sw}$ = Concentration of Labp is soil water in layer. (kg/m^3)

q_{mat} = Amount of matrix flow percolating out of a soil layer. (m)

K_d = Soil partitioning coefficient (m3/kg)

m_s = Mass of a soil layer. (kg/m^2)

SW = Soil water content of the soil layer. (m)

$$C_{labp,SW} = \frac{LabP}{K_d m_s + SW} \tag{119}$$

$$K_d = 0.1 + 0.25\ clay \tag{120}$$

Where, Labp = P in labile P pool of a soil layer. (kg/m^2)

Clay = Clay fraction of a soil layer. (-)

Amount of DRP loss from first soil layer is added to labile P pool of the next soil layer and so on until it reaches the groundwater reservoir and added to it.

In case of DRP loss through macropore flow, It is assumed that macropore flow occurs as a short-circuit flow i.e. it is originated from the first soil layer and directly contributes to the groundwater reservoir. Amount of P leached out by the macropore flow is calculated as (Steenhuis et al., 1994).

$$P_{leach,mac} = C_{labp,SW,1}\left(1 - \exp\left(\frac{-R}{K_{d1}m_s 1 + SW_1}\right)\right) * r \tag{121}$$

Where, $P_{leach,\ mac}$ = Amount of DRP loss through macropore flow. (kg/m^3)

R = Rainfall amount (m)

r = ratio of macropore flow to the total flow from the first soil layer. (-)

$$r = \frac{V_{mac}}{V_{mac}+V_{mat}} \tag{122}$$

Where, V_{mac} = Volume of macropore flow. (m^3)

V_{mat} = Volume of matrix flow. (m^3)

1 in subscripts stands for all the variables as defined above for the first soil layer only.

DRP loss from the groundwater reservoir is calculated by mass balance approach. i.e.

Change in P mass in GW reservoir = Incoming P mass – Outgoing P mass

$$y'(t) = I_{drp} - \frac{y(t)}{S_{gw}} * drain \tag{123}$$

Where, y(t) = Mass of DRP present at any time t in the groundwater reservoir. (kg)

I_{drp}= Incoming DRP mass to groundwater reservoir through macropore and matrix flow. (kg)

S_{gw} = Storage volume of the groundwater reservoir during time t. (m^3)

Drain = Outflow volume from the groundwater reservoir i.e. the tile drainage amount. (m^3)

t = time. (days)

By solving equation 123 we get

$$y(t) = \frac{S_{gw} * I_{drp}}{drain} + \left(y_0 - \frac{S_{gw} * I_{drp}}{drain}\right) * \exp\left(-\frac{drain}{S_{gw}} * t\right) \quad (124)$$

In case of Drain = 0 then

$$y(t) = I_{drp} * t + y_0 \quad (125)$$

Where, y_0 = initial amount of P mass in the groundwater reservoir at the beginning of the day. (kg)

Average concentration of DRP in 1 day the groundwater reservoir

$$C_{drp,gw} = \frac{y_0 + y(1)}{2 * S_{gw}} \quad (126)$$

Where, $C_{drp,gw}$ = Concentration of DRP in groundwater reservoir. (kg/m^3)

The mass of DRP loss through tile drainage is calculated as

$$Drplosstdrain = C_{drp,gw} * drain \quad (127)$$

Where, Drplosstdrain = Mass of DRP loss through tile drainage. (kg)

A11 PP LOSS TILE DRAINAGE

PP loss through tile drainage is based on the model described by Jarvis et al., (1999). In this approach it is assumed that PP loss through tile drainage only happens through macropore flow and originates only from the first soil layer. The macropore flow along PP is added to the groundwater reservoir then it finally loss through tile drainage with drainage water.

Soil detachment is calculated as

$$D = K_d * E * R * M_s * Crop \tag{128}$$

Where, D = Detachment of soil particle. (gm m^{-2} day^{-1})

K_d = Soil detachability coefficient. (gm J^{-1})

E = Kinetic energy of the rain. (J m^{-2} mm^{-1})

R = Rainfall rate. (mm day^{-1})

M_s = Amount of readily available dispersible particle (gm gm^{-1} soil)

Crop = An empirical crop management factor used in USLE for reduction in particle detachment when the crop covers the soil.

$$Crop = 1 - FC * \exp(-0.34H) \tag{129}$$

Where, H = effective canopy height (m)

FC = fraction of land surface covered by crop canopy. (-)

$$H = 0.6 * \text{crop height} \tag{130}$$

$$FC = 6.5 * LAI^{0.75} * S^{-0.48} \tag{131}$$

Where, LAI = leaf area index. (-)

S = row spacing. (mm)

E depends upon the amount of rainfall and it is calculated as

$$E = 29 * (1 - 0.72\exp(-0.05R)) \tag{132}$$

The value of M_s dynamically changes due to particle replenishment. In case of just after tillage, if the M_s does not reached 50% of its maximum value (M_{smax}) then the model make it 50% of its maximum value. M_{smax} is calculated as

$$M_{smax} = 0.362 * clay - 0.518 \tag{133}$$

Where clay = clay content of the soil (%)

If we do mass balance of the available particle at the soil surface (A_s) then

$$\frac{dA_s}{dt} = -D + P \tag{134}$$

Where, P is the particle replenishment. It is calculated as

$$P = K_r(1 - \frac{M_s}{M_{smax}}) \tag{135}$$

Where, K_r = Replenishment rate coefficient. (gm m^{-2} day^{-1})

$$A_s = M_s * \gamma * Z_d \tag{136}$$

Where, γ = Bulk density of the surface soil layer. (gm/m^3)

Z_d = Depth of the surface soil layer. (m)

Now, substituting the value of P, A_s and D in the equation 135 then solving it for M_s we get

$$M_s = \frac{1}{K}\left(K_r + (KM_{so} - K_r) * \exp\left(-\frac{Kt}{\gamma Z_d}\right)\right) \tag{137}$$

$$K = K_d * E * R * Crop + \frac{K_r}{M_{smax}} \tag{138}$$

Where, M_{so} = Initial amount of M_s before the beginning of a day.

t = time (1 day)

Concentration of suspended particle routed into the macropore flow is calculated as

$$C_{sp,mac} = \frac{D}{R+Z_d SW_1} \tag{139}$$

Where, $C_{sp,mac}$ = Concentration of suspended particle routed into the macropore flow

(gm m^{-2} mm^{-1})

R = Rainfall (mm)

Z_d = Depth of the surface soil layer. (mm)

SW_1 = Soil water content of the surface soil layer. (m^3/m^3)

Due to filtering, the mass of suspended particle reaching the groundwater reservoir decreases as follows

$$M_d = q_{mac} * C_{sp.mac} * \exp\left(-f * d_{gw}\right) \tag{140}$$

Where M_d = Mass of suspended particle reaching the groundwater reservoir. (gm m^{-2})

f = filter coefficient (m^{-1})

d_{gw} = Depth to groundwater reservoir. (m)

Mass of PP reaching groundwater reservoir is calculated as

$$M_{pp} = f_{md} * (Labp(1) + ActP(1) + Stabip(1) + Frsop(1) + Stabop(1) + Manwip + Manwop + Mansip + Mansop + Avfertp + Resfertp) \tag{141}$$

Where, M_{pp} = Mass of PP reaching groundwater reservoir (kg/ha)

f_{md} = A factor

$$f_{md} = \frac{M_d}{\gamma Z_d} \tag{142}$$

Where, γ = Bulk density of the first soil layer. (gm/m^3)

Z_d = Depth of the surface soil layer. (m)

PP loss from groundwater reservoir through tile drainage is calculated by mass balance approach

Change in PP mass in groundwater reservoir = Incoming PP mass – Outgoing PP mass i.e.

$$\frac{dy}{dt} = I_{pp} - \frac{y(t)}{S_{gw}} drain \tag{143}$$

Where, y(t) = Mass of PP present at any time t in the groundwater reservoir. (kg)

I_{pp}= Incoming PP mass to groundwater reservoir through macropore flow. (kg)

S_{gw} = Storage volume of the groundwater reservoir during time t. (m^3)

Drain = Outflow volume from the groundwater reservoir i.e. the tile drainage amount. (m^3)

t = time. (days)

Solving equation 144 we get

$$y(t) = \frac{S_{gw}}{drain} * I_{pp} + \left(y_0 - \frac{S_{gw}}{drain} * I_{pp}\right) * \exp\left(-\frac{drain}{S_{gw}} * t\right) \tag{144}$$

In case of drain =0

$$y(t) = I_{pp} * t + y_0 \tag{145}$$

Where, y_0 = initial amount of PP mas in the groundwater reservoir at beginning of the day. (kg)

Concentration of PP in groundwater reservoir in a day is calculated as

$$C_{pp,Gw} = \frac{y_0 + y(1)}{2 * S_{gw}} \quad (146)$$

Where, $C_{pp,gw}$ = Concentration of PP in groundwater reservoir. (kg/m^3)

Amount of PP loss through tile drainage is calculated as

$$PPlosstdrain = C_{pp,gw} * drain \quad (147)$$

Where, PPlosstdrain = Mass of PP loss through tile drainage. (kg)

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