

Article

Development and Validation of a Crop and Nitrate Leaching Model for Potato Cropping Systems in a Temperate–Humid Region

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Abstract: The Root Zone Water Quality Model (RZWQM) is a one-dimensional process-based model used for simulating major physical, chemical, and biological processes in agricultural systems. To date, the model has not been applied to potato production systems for simulating nitrate leaching. In this study, 35 datasets collected between 2009 and 2016 at a field under a three-year potato (potato–barley–red clover) rotation in Prince Edward Island (PEI), Canada, have been employed for calibrating and validating the water, nitrogen (N) cycling, and plant growth routines of RZWQM and for subsequently estimating nitrate leaching. The model fitness, evaluated using univariate and bivariate indicators, was rated as high for most of the parameters tested. As a result of the combined influence of higher infiltration and reduced plant uptake, the model showed that the highest leaching at the rotation level occurred between September and December. A secondary leaching period occurred in spring, when residual soil nitrate was mobilized by increased percolation due to snow-melt. Most of the nitrate leaching occurred during the potato year (89.9 kg NO₃-N ha⁻¹ y⁻¹), while leaching for barley and red clover years had comparable values (28.6 and 29.7 kg NO₃-N ha⁻¹ y⁻¹, respectively). The low N use efficiency of the entire rotation (i.e., 30.2%), combined with the high NO₃-N concentration in leachate (i.e., 34.9 mg NO₃-N L⁻¹ for potato and 16.3 mg NO₃-N L⁻¹ for the complete rotation), suggest that significant efforts are required for adapting management practices to ensure sustainability of potato production systems.

Keywords: nitrate leaching; crop modelling; RZWQM; agricultural drainage; sustainability of agricultural systems; groundwater contamination

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1. Introduction

Potato is the fourth most important food crop in the world [1]. Long-term global increases in both potato acreage and yield have been recorded in the last several decades [2,3], and this trend is expected to continue in the future [4,5]. In Canada, potato production is concentrated in Alberta (21.8% of total production), Prince Edward Island (21.6%), and Manitoba (21.3%) [6]. For Prince Edward Island (PEI), an island with a humid temperate climate, potato is the most important agricultural commodity, with land in potato

rotation representing about 18.3% of PEI's landmass [7]. Potato cropping systems in PEI have been associated with an increased concentration of nitrate in groundwater [8–10], and this has been linked to an increased frequency of hypertrophic and anoxic conditions in coastal waters [11–13]. Similar findings have been reported in many other areas of the world where intensive potato cropping systems are in place [14–16]. Considering the importance of the potato industry for the provincial economy and environment, potato cropping in PEI is regulated as a three-year rotation cycle, a practice aimed at reducing the risk of nutrient losses and soil erosion [17,18]. The most common potato rotation in PEI is potato–barley–red clover (PBC), and the most popular potato variety is Russet Burbank [18,19], which is also the most widely grown potato variety in North America [20]. The Russet Burbank variety is the french fries processing industry standard, with high yield and quality, excellent storability, and resistance to a series of diseases; however, it has low nutrient uptake efficiency [1]. Barley is underseeded with clover to help regenerate the soil in the two years following potato harvest.

Agricultural production and the environment are interlinked as agricultural practices can impact soil and water quality, while environmental factors such as climate and soil properties can also impact agricultural production. Soil–crop models simulate crop growth and soil–plant system dynamics in conjunction with climate and agricultural practices and are suitable for simulating soil N cycling and crop yield, and they are often used to model nitrate leaching [21–23]. These models can be further used to develop scenarios for analyzing the effects of modifying agricultural practices (e.g., fertilizer application rate and timing, irrigation) or changing climate. The Root Zone Water Quality Model (RZWQM) [24,25] is a complex one-dimensional modelling system developed by the United States Department of Agriculture (USDA) that integrates plant growth, water movement, chemical transport, and soil N and carbon cycles to allow for simulation of the physical, chemical, and biological processes in the root zone, and thus for evaluation of the impact of agricultural management systems on crop productivity and environmental quality [26–28]. RZWQM incorporates several methods and models that are considered standards for simulating various relevant processes such as the Brooks–Corey functions [29] for describing soil moisture parameters, the Richards equation [30] for movement of water in unsaturated soils, and DSSAT [31] and HERMES [32] for plant growth. Despite its popularity, to the best of the authors' knowledge, to date, there are no previous studies that have utilized RZWQM to investigate nitrate leaching for potato cropping systems.

Several previous studies have investigated the dynamics and magnitude of nitrate leaching, or other soil N budget terms, for potato cropping systems in PEI. However, these studies typically did not integrate crop growth modelling and used limited calibration and validation datasets, with the estimates being obtained via a mix of modelling and in situ measurements. For example, Jiang et al. (2011) [33] employed LEACHN [34] in combination with MODFLOW [35] to simulate long-term (1999–2008) nitrate leaching from a PBC rotation in PEI using a study site located at AAFC's Harrington Experimental Farm (HEF). Liang et al. (2019) [36] used statistical approaches in combination with measured soil water nitrate concentrations and plant N content to estimate the N surplus for a PBC rotation at HEF. Jiang et al. (2022) [19] used soil, soil water, and plant tissue data collected from fields located at HEF in combination with LEACHN and statistical approaches to estimate nitrate leaching and tuber yield response to different crop rotations. Only a couple of previous PEI studies employed plant-growth modelling for potato cropping systems; however, these studies are generally covering only the growing season, for a reduced number of years, had limited experimental data, and did not include estimates of potato yield or nitrate leaching. Using data collected from one growing season (i.e., 2012), Morissette et al. (2016) [23] developed a soil–crop model for the potato variety Shepody using the STICS soil–crop generic model [37] to assess the ability of the model to predict potato yield and N uptake for a range of N fertilization scenarios. Adekanmbi et al. (2023) [38] used the Decision Support System for Agrotechnology Transfer model (DSSAT) [31] to study the effects of future climate changes on potato yield.

The study is part of a larger effort led by AAFC and ECCC to advance the knowledge of the linkages between intensive agricultural practices and groundwater quantity and quality, while ensuring the environmental and economic sustainability of these practices. In this context, our study is aimed at understanding the potential of current agricultural practices associated with potato cropping for releasing excess nutrients to the subsurface environment, while also evaluating the efficiency of N use for the typical potato rotation systems in PEI. Using a PBC rotation, the objectives of the study were to i) use RZWQM to develop a robust crop model for each phase of the rotation using a multifaceted calibration and validation procedure; ii) estimate the magnitude, and inter- and intra-annual variation of the nitrate leaching associated with the rotation; and iii) evaluate the N use efficiency of the rotation. Specifically for PEI, the study addresses several knowledge gaps including the lack of nitrate leaching estimates obtained using plant-growth models, the often limited field-based datasets used to produce nitrate leaching estimates when alternative modelling approaches were involved, and the limited studies available for evaluation of N use efficiency. While the study is representative of the agricultural practices and landscape conditions of PEI, it is also relevant for other intensive potato cropping areas, particularly in temperate–humid climates, as generally the previous studies were limited to discontinuous results limited to the growing season. The model developed as part of this research will also allow for development and testing of scenarios relevant to the impact of, for example, fertilizer management, irrigation, and climate change on both plant growth and environmental fluxes.

2. Materials and Methods

2.1. Site Description

AAFC Harrington Experimental Farm (HEF) (46°20'34" N, 63°09'50" W) is an experimental research farm belonging to AAFC, situated about 11 km north of Charlottetown, PEI, in Atlantic Canada (Figure 1). The climate in the area is temperate and humid, with an average annual air temperature of 5.7 °C. The minimum monthly average air temperature is −7.7 °C (January), while the maximum monthly average is 18.7 °C (July) [ECCC 2021]. The average annual precipitation, which is relatively uniformly distributed during the year, is 1150 mm, with 25% occurring as snow. The snowpack reaches a maximum depth of 30 cm in February and typically leads to significant snowmelt periods between February and April [39]. The soils at HEF belong to the Charlottetown soil association and have a sandy loam texture, being classified as an Orthic Humo-Ferric Podzol according to the Canadian system of soil classification [40]. The Charlottetown soil association is the dominant soil in the province and is representative of the soils used for potato production in PEI [40,41]. These soils are generally well drained; however, due to the lower permeability of the underlying glacial till, transient perched water can occur for several days per year following snowmelt [18,42].

2.2. Experimental Field Setup

The monitoring and sampling program took place in Field 355 (Figure 1), which is positioned on a gentle slope oriented in the NW–SE direction. The field has been under a potato [*Solanum tuberosum* L.]—barley [*Hordeum vulgare* L.]—red clover [*Trifolium pratense* L.] (PBC) 3-year potato rotation since 2009. The field has been divided into three sections (Section A, 2.4 ha; Section B, 0.7 ha; and Section C, 0.6 ha) using a 3 (phases) by 3 (sections) experimental design (Figure 1, Table 1). Thus, each rotation phase was present in one section of the field in any given year. For the purpose of data analysis, the red clover was separated into Red Clover 1 (RC1), which included the red clover present in the field in the barley year (i.e., year two of the rotation; emergence following the barley harvest) and Red Clover 2 (RC2), which represented the red clover present in the field in the clover year (i.e., year three of the rotation). Most of the instrumentation was located in Section A, with data collected between 2009 and 2016 from this section used for the calibration of the

RZWQM model. Data collected from section B during the same period were used for validating the performance of the calibrated model.

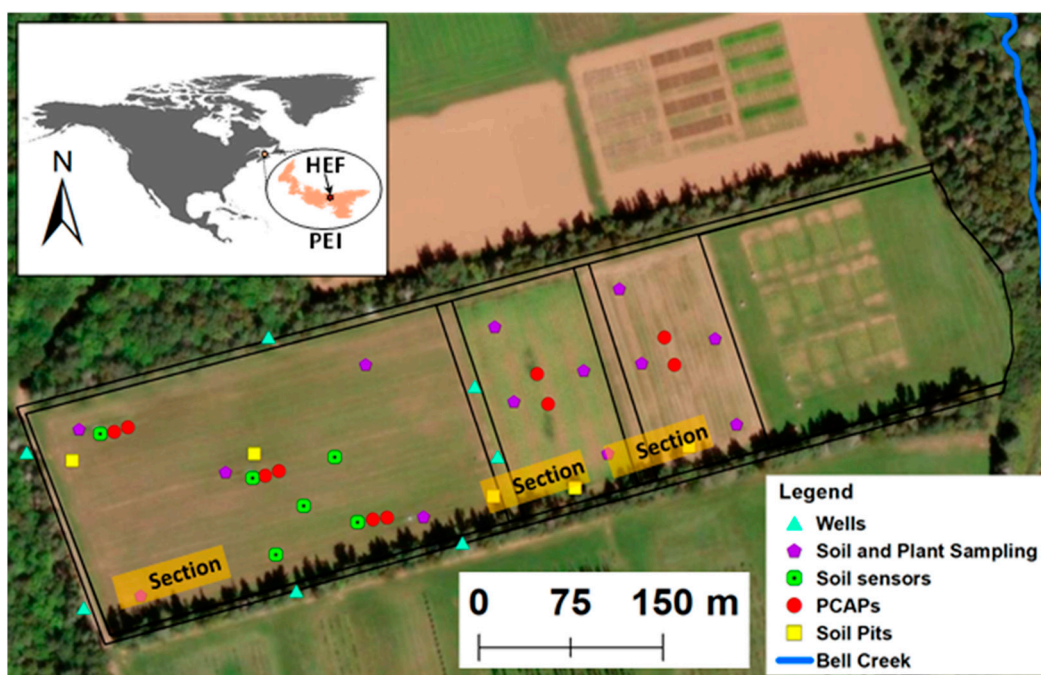


Figure 1. Monitoring and sampling locations in Field 355 and the location of the study site (inset).

Table 1. Crop rotation phases for Sections A and B of Field 355.

Year	Section A	Section B
2009/10	Barley (16 May 2009 to 30 August 2009) underseeded with RC1 (31 August 2009 to 27 May 2010)	RC2 (28 May 2009 to 18 May 2010)
2010/11	RC2 (28 May 2010 to 29 May 2011)	Potato (19 May 2010 to 25 May 2011)
2011/12	Potato (30 May 2011 to 27 May 2012)	Barley (26 May 2011 to 25 August 2011) underseeded with RC1 (26 August 2011 to 27 May 2012)
2012/13	Barley (28 May 2012 to 30 August 2012) underseeded with RC1 (31 August 2012 to 27 May 2013)	RC2 (28 May 2012 to 6 May 2013)
2013/14	RC2 (28 May 2013 to 29 May 2014)	Potato (7 May 2013 to 29 May 2014)
2014/15	Potato (30 May 2014 to 27 May 2015)	Barley (30 May 2014 to 26 August 2014) underseeded with RC1 (27 August 2014 to 27 May 2015)
2015/16	Barley (28 May 2015 to 2 September 2015) underseeded with RC1 (3 September 2015 to 24 May 2016)	RC2 (28 May 2015 to 24 May 2016)
2016	Barley (25 May 2016 to 2 September 2016)	Barley (25 May 2016 to 2 September 2016)

Potatoes (cultivar Russet Burbank) were planted between mid-May and early June at a rate of $\sim 2700 \text{ kg ha}^{-1}$ cut seed and seeded with a machine with 0.91 m and 0.31 m row spacing and seed spacing, respectively. Banded NH_4NO_3 inorganic fertilizer (150 kg to 170 kg N ha^{-1}) was applied at the time of planting. Phosphorus and potassium fertilizer were also applied with N fertilizer as recommended [43]. Fungicides and herbicides were applied according to standard grower practice. Harvesting occurred between the end of October and early November, with the potatoes top-killed with a desiccant herbicide applied four and two weeks before harvest. Barley (var. Island) was planted at a 150 kg ha^{-1} seeding rate and was underseeded with red clover (var. Charlie) at a 12 kg ha^{-1} seeding rate. NH_4NO_3 inorganic fertilizer (51 kg N ha^{-1}) in combination with P (as Triple superphosphate) and K (as muriate of potassium) fertilizers were applied at the time of planting, and herbicide was applied post-emergence. The barley was harvested between the end of August and the beginning of September, and the straw was removed from the field. The

red clover was cut two to three times, with the last cut occurring between the end of October and mid-November. The red clover was flailed and mowed, and the residues were left in the field. A complete description of the agricultural management operations is provided in Supplementary Material S1.

2.3. Datasets

The complete dataset used for the calibration and validation of the RZWQM model is presented in Supplementary Material S2.

2.3.1. Meteorological Data

Daily meteorological data between 2009 and 2016, used as input for RZWQM, included precipitation, minimum and maximum air temperature, wind speed, and relative air humidity and were obtained from an Environment and Climate Change Canada Charlottetown weather station (46°17'24" N, 63°7'48" W) [44]. Because a complete local dataset for shortwave solar radiation (SR) was not available, this was obtained from NASA—The Power Project database [45], based on the geographical coordinates of the Charlottetown weather station. The dataset obtained from NASA had a very good correlation with a short-term (2014) dataset available from the local weather station ($SR_{LOCAL} = 0.975 \times SR_{NASA}$; $r^2 = 0.94$), and hence, the use of the NASA dataset for this study was considered appropriate. Snowfall and snowpack depth obtained from the Charlottetown weather station were used for calibrating the output from the RZWQM routines related to snowfall, snow accumulation, and snowmelt.

2.3.2. Soil Water Content and Temperature

Soil water content (SWC), temperature, and electrical conductivity were logged hourly between 2010 and 2019 using 5TE Decagon sensors connected to EM50 data loggers (METER Group, Pullman, WA, USA). The measurements were conducted at up to 6 locations in Section A (Figure 1), with the sensors installed at four or five depths at each location, with depths ranging from 5 to 80 cm below the ground surface. Detailed procedures regarding the installation of the sensors and processing of data collected are presented in Danielescu et al. (2022) [3]. Data collected from the various locations were averaged to obtain daily SWC and temperature time series that were used for calibration of the water budget components of RZWQM.

2.3.3. Drainage and Nitrate Leaching

The quantity and quality of the water leaving the soil profile was sampled using Passive Capillary Samples (PCAPs) (Figure 2). A total of 8 PCAPs (6 in Section A and 2 in Section B) were installed at 60 cm below the ground surface and were sampled on a monthly basis. The sampling was less frequent during summer, due to the limited amounts of drainage water, and occasionally more frequent during spring, when increased drainage led to two sampling dates per month. PCAPs consist of plastic bins with a maximum capacity of ~300 L (0.8 L × 0.45 W × 0.8 H m), with 6 clusters of fiberglass wicks placed at the top of each PCAP lid (Figure 2). PCAPs were constructed on-site by adapting the design proposed by Louie et al. (2000) [46] and Jabro et al. (2007) [47]. The bins were buried in the field, and underground sampling lines were installed through 3" PVC pipes, with sampling ports located in areas where they would not interfere with agricultural operations (i.e., sampling nests). The sampling ports were raised to about 60 cm aboveground so they were accessible during the winter months (Figure 2).

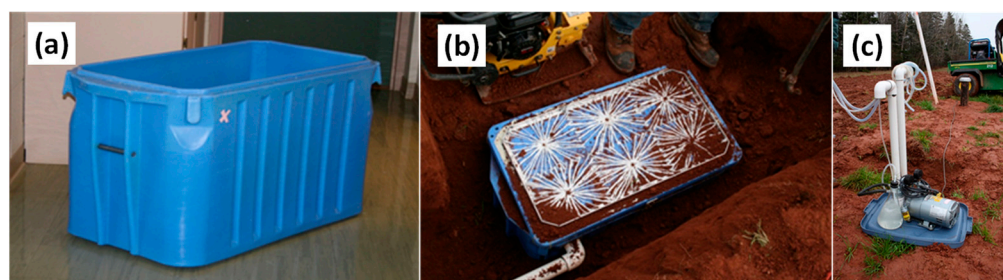


Figure 2. Design, installation, and sampling setup for the Passive Capillary Samplers (PCAPs) at the study site: (a) PCAP plastic bin used as PCAP collection tank; (b) installation of the PCAP showing the bin top with perforated wicks; (c) sample collection ports after installation completion.

At each sampling, the PCAPs were completely emptied using a 0522-V48B Gast vacuum pump (Gast Manufacturing Inc., Benton Harbor, MI, USA), and the total volume collected was measured with graduated containers. The samples were refrigerated (i.e., <4 °C) in 50 mL HDPE bottles until analyzed. The samples were analyzed at AAFC's Charlottetown Regional Lab using a QuikChem 8500 flow injection analysis system (Lachat Instruments, Loveland, CO, USA) for nitrate and ammonium, with a method detection limit of 0.025 mg N L⁻¹.

The ammonium concentration was very low or below the detection limit for the majority of the drainage samples. Consequently, ammonium in drainage samples was not considered in this study. The nitrate concentrations associated with each sampling date were considered to be representative of the period extending to the previous sampling date. The average nitrate concentration for each section and sampling date was calculated as the average nitrate concentration in all PCAPs in the respective section, weighted by the volume of water collected in each of the PCAPs.

Nitrate leaching was obtained as the product of nitrate concentrations and drainage volume. Daily time series for both nitrate concentrations and drainage were built to calculate the daily nitrate leaching. The daily nitrate concentration series was obtained by using the volume-weighted average nitrate concentration measured in PCAPs at each sampling date as a representative value for each day between the respective sampling date and the previous sampling date. The cumulative annual water volumes collected by each PCAP exceeded the annual precipitation two- to threefold, and hence, these were not used for the calculation of daily drainage. The excessive amount of water collected by the PCAPs was attributed to either the transient perched water conditions present at the site [42] and/or to the inadequate wick calibration during the PCAPs' design [48,49]. Instead, the daily drainage output obtained with the SNOSWAB (Snow, Soil Water and Water Balance) model [50] was used (Supplementary Material S3).

2.3.4. Soil Sampling

Five soil pits (~ 4 m L \times 1.5 m W \times 1 m D) were dug in October 2009 across Section A. The depth of soil horizons, depth to the underlying till, and root layer depth were determined. Disturbed and undisturbed samples were collected and analyzed following the procedures described in Danielescu et al. (2022) [3] for the determination of bulk density, porosity, texture, hydraulic conductivity, and organic matter content. Soil water content (SWC) at various matric potentials was measured using tension tables at -0.5 , -5 , and -10 kPa and pressure plates at -33 and -100 kPa, using the procedure described by Topp and Zebchuk (1979) [51]. The soil properties for each horizon were consistent for all locations, and hence, the values obtained for each parameter in each of the soil horizons of each pit were averaged to obtain a representative value for the entire field. Soil properties were used for parametrizing the Horizon Description, Soil Hydraulics, and Soil Physical properties of the RZWQM model, including for the parametrization of the Brooks–Corey model [29].

Soil sampling was carried out once before seeding, once in late-fall and up to four times during the summer and early fall, and the samples were analyzed for nitrate, ammonium, organic matter, total carbon, and total N at AAFC's Charlottetown Regional Lab. Soil samples were collected at 15 cm depth intervals to a maximum depth of 60 cm, using either a Dutch auger or a hydraulic core sampler (Giddings Machine Company, Windsor, ON, Canada), from five locations in Section A and four locations in Section B, and for each sampling location, three to four subsamples were bulked together to constitute one composite sample for each depth. Mineral N was extracted on moist soil using the KCl extraction method [52]. The extracts were analyzed for nitrate and ammonium concentrations by flow injection analysis (FIA) using a Lachat QuikChem 8500 system (Lachat Instruments, Loveland, CO, USA). A portion of the soil sample was air-dried, sieved through 2 mm and ground to pass a 0.25 mm sieve, and analyzed for total carbon and total nitrogen concentrations using the dry combustion method on an Elementar Vario Max analyzer (Elementar Analysensysteme GmbH, Langenselbold, Germany). The nitrate and ammonium concentrations were converted into N equivalent concentrations and transformed into soil nitrate and ammonium content for the various depths. The total inorganic soil N was calculated as the sum of nitrate and ammonium content, and the average for each sampling date was calculated as the average of the samples collected from each location. Soil properties were used for the parametrization of the RZEWQM model, while nitrate and ammonium content were used for calibrating the N cycling components of the RZWQM model.

2.3.5. Plant Tissue Sampling

Aboveground plant tissue samples for all phases of rotation were collected using a 1 m² quadrant for dry matter content, total C and N concentrations, and C:N ratio analyses. Samples were collected from five locations in Section A and four locations in Section B, and for each sampling location, three to four subsamples were bulked together to obtain a composite sample. For the legume phase (red clover), the plants were sampled up to three times per season (mid-June, mid-August, and before plowing down) shortly before cutting. Barley was sampled once at the end of July, when the crop started to mature, and once at the end of August, at harvest. The barley plant was analyzed as a whole for the first sampling date, whereas for the second sampling date, the kernel and straw were analyzed separately. Potatoes were sampled two to three times per season, and tubers, vines, and stolons were analyzed separately. Sampled plant tissues were weighed to determine wet biomass, and a subsample (200 g to 300 g) was oven-dried at 55 °C for dry matter content analysis. Air-dried plant tissue samples were ground to pass a 1 mm screen with a Wiley Mill grinder (Arthur H. Thomas Co., Philadelphia, PE, USA) and thereafter analyzed for total C and N content using an Elementar Vario Max analyzer (Elementar Analysensysteme GmbH, Langenselbold, Germany). The data obtained from plant tissue sampling were used for calibration of the RZWQM crop submodels for each phase as well as for the calibration and validation of the output from the N cycling components of the model.

2.4. RZWQM Setup

Separate daily timestep simulations were developed for Section A and Section B, to allow for calibration (Section A) and the validation of the calibrated model (Section B), respectively. The simulated period encompassed slightly more than two full PBC rotations (i.e., 7 years; 2009–2016). To ensure representative initial conditions for the simulations, the data collected between 2009 and 2016 were duplicated and added to the model simulations as a “warm up” period (2001–2008). Unless specified, the default values available in RZWQM were left unchanged. Three soil layers were defined in the model (i.e., 0–20 cm, 20–40 cm, and 40–60 cm depth), with the bottom boundary of the deepest layer corresponding to the depth of the installation of the PCAPs. Data obtained from the soil surveys and soil sample analysis were used for parametrization of the horizon description and soil hydraulics components of the model. The initial values for various

humus/organic matter pools (e.g., slow and fast residue; slow, intermediate, and fast humus; aerobic and anaerobic heterotrophs; autotrophs) were estimated using the Initialisation Wizard built into RZWQM. The Nutrient Pool Equilibration routine of RZWQM was used with study site data (e.g., temperature range, duration of the growing season) for 50 years to estimate the initial residue pools. Daily measured meteorological data were imported into RZWQM for creating the model-required meteorology files.

The red clover crop in the rotation was simulated using alfalfa [*Medicago sativa* L.] because, in RZWQM, this crop has the plant growth model fully implemented in RZWQM and allows for simulation of multiple cuts throughout the growing season. This was considered reasonable, as previous studies show that mineral soil N content [53] and N fixation rates [54,55] are similar for the two species. The potato plant was simulated using the Russet Burbank cultivar, and barley was simulated using the high-latitude barley variety, both available in the RZWQM database. Additional agricultural management information was added to RZWQM based on the data collected from the field (Supplementary Material S1, Supplementary Material S2). This information included crop (e.g., date of planting, planting depth, method of planting, and date of harvesting), fertilization (date, method, and rate of fertilizer application as well as $\text{NO}_3\text{-N}$ and $\text{NH}_4\text{-N}$ content of fertilizer), pesticides (pesticide name, date of application, method of application, and amount), and tillage (timing of operation, type of tillage implement, and depth of tillage data).

A complete description of the information entered into the various modules of RZWQM for the parametrization of the model is included in Supplementary Material S4. The N soil budget equations as integrated in RZWQM are included in Supplementary Material S5.

2.5. RZWQM Calibration and Validation

The objective of the calibration (Section A, 2009–2016) was to achieve a moderate or high fit between simulated and calibration data with respect to soil water, N cycling, and plant growth components of the model, with a particular focus on nitrate leaching and crop yield. During the RZWQM parametrization, 97 model parameters (i.e., constants) were changed based on existing field data. The complex calibration procedure involved 35 calibration datasets (Supplementary Material S2) and adjustment of 61 parameters (Supplementary Material S4), when all phases of the rotation were considered (i.e., potato, barley, and red clover with the RC1 and RC2 subcomponents).

The calibration was conducted by inverse modelling using the RZWQM built-in Parameter Estimation (PEST) routines [25,56] combined with trial and error for minimizing the differences between the field calibration data and the output for various components of RZWQM. The trial-and-error procedure was employed as the PEST routines incorporated in the current version of RZWQM include only several RZWQM components, and within each of these components, only a subset of the parameters and variables required for running the model were available. The performance was assessed using univariate (e.g., average) and bivariate statistics (i.e., R^2 —coefficient of determination, NRMSE—Normalized Root-Mean-Square Error, PBIAS—Percentage Bias) (Equation (1) to Equation (3)) for various time steps and averaging intervals. The averaging intervals included monthly, yearly, calendar season, crop phase, and crop year. In addition, values for corresponding “typical” intervals were calculated across all the periods when a crop was present in the field (e.g., the typical average value for potato nitrate leaching for the month of July was obtained by averaging all the July months during the simulation period when the potato plant was present in the field). The model performance rating scheme for the bivariate statistics is shown in Table 2. R^2 rating intervals were based on Cohen (1988) [57], while for NRMSE and PBIAS, they were based on Moriasi et al. (2007) [58]. A larger PBIAS was allowed for N cycling and crop components to account for the increased complexity of these components of the model.

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^n (Y_{i\text{ME}} - Y_{i\text{MO}})^2}{n}} \quad (1)$$

where

RMSE—Root-Mean-Square Error

$Y_{i\text{ME}}$ —the i th measured value (i.e., observed)

$Y_{i\text{MO}}$ —the i th value predicted by the model (i.e., modelled)

n —number of available data points.

$$\text{NRMSE} = \frac{\text{RMSE}}{Y_{\text{ME_MAX}} - Y_{\text{ME_MIN}}} \quad (2)$$

where

NRMSE—Normalized Root-Mean-Square Error

$Y_{\text{ME_MAX}}$ —maximum measured value (i.e., observed)

$Y_{\text{ME_MIN}}$ —minimum measured value (i.e., observed)

$$\text{PBIAS} = \frac{\sum_{i=1}^n (Y_{i\text{ME}} - Y_{i\text{MO}})}{\sum_{i=1}^n Y_{i\text{ME}}} \times 100 \quad (3)$$

where

PBIAS—Percentage Bias (%)

$Y_{i\text{ME}}$ —the i th measured value (i.e., observed)

$Y_{i\text{MO}}$ —the i th value predicted by the model (i.e., modelled)

Table 2. Ranges of values of statistical indicators used for evaluation of model fitness.

Statistics	Best Case Value	Model Fitness		
		Low	Moderate	High
R^2	1	<0.3	0.3 to 0.5	>0.5
NRMSE	0	>0.7 (>70%)	0.5 to 0.7 (50 to 70%)	<0.5 (<50%)
PBIAS (water)	0	<-50% or >50%	-50% to -25% or 25% to 50%	-25% to 25%
PBIAS (N cycle and crop)	0	<-70% or >70%	-70% to -50% or 50% to 70%	-50% to 50%

The calibration data were obtained via direct measurements, derived from the literature, or obtained from secondary modelling. The calibration procedure involved adjusting various RZWQM model parameters to improve the fit between the model output and the calibration data. The calibration data were separated into discrete (i.e., data available only for the sampling dates) and continuous (i.e., daily) datasets. Discrete datasets included soil physical properties (e.g., porosity, texture, water retention curve); soil inorganic N; aboveground, belowground, and total biomass; plant uptake; N content in plant tissue; C/N ratio in plant tissue and soil; aboveground dry weight; potato tuber fresh yield; potato vine, tuber, and stolon dry weight; red clover N fixation. Continuous datasets included soil water content and temperature, meteorological data, and data derived from secondary modelling. In addition, N concentration in soil water, collected at various dates (i.e., discrete data) using PCAPs, was converted to a continuous dataset. For the potato phase, an additional application of fertilizer was incorporated in the model during the fall, to compensate for the limited ability of the model to simulate the high peaks in nitrate concentration and leaching observed in the measured data. The fall peak in leaching, as well as the challenges associated with its simulation, were noted by other authors in the past [18,33,36]. The amount of fertilizer added during the fall was set to the same amount of nitrogen contained in post-harvest plant residue (i.e., 34.9 kg N ha⁻¹ in 2011 and 36.7 kg

N ha⁻¹ in 2014). In addition, the harvest efficiency for potato was increased to 90% to minimize the amount of residue left in the field after harvest. The complete list of calibration data used is included in Supplementary Materials S2 and S4.

Secondary modelling involved the use of additional models for deriving several daily datasets required for RZWQM calibration. These models were all part of the Hydrology Tool Set (HTS) online suite of tools [59]. Percolation, snow depth, and snowmelt were estimated using SNOSWAB (Snow, Soil Water and Water Balance Model) [50]. The details of the calibration procedure for SNOSWAB are included in Supplementary Material S3. Surface runoff was obtained with eleven hydrograph separation algorithms included in SepHydro [60]. Considering differences in surface runoff generation at watershed scale vs. field scale and the absence of data from other sources, this was considered a reasonable approach at least at larger temporal scales (e.g., monthly basis). The details of the calibration procedure for SepHydro are included in Supplementary Material S6. Actual evapotranspiration for the entire study period was estimated using eight methods included in ETCalc and used the same dataset as presented in Danielescu (2023c) [61]. Evapotranspiration estimation methods were calibrated such that the multi-annual average of actual evapotranspiration was similar to the values previously reported in the literature [62].

Validation of the model (Section B, 2009–2016) was conducted to assess if the model accurately represents the PBC rotation for the site conditions. The validation datasets included Section B values for the parameters and variables used for the calibration of the model. Similar to the calibration simulation, an additional application of fertilizer was incorporated into the model during the fall of the potato phase (i.e., 37.9 kg N ha⁻¹ in 2010 and 19.5 kg N ha⁻¹ in 2013), and the settings of the model were adjusted accordingly. Testing of the fitness between the validation simulation output and the validation datasets used the same procedure as for the calibration simulation. The complete list of validation data used is included in Supplementary Materials S2 and S4.

3. Results and Discussion

3.1. Model Calibration

When considering the various averaging periods for the continuous datasets, NRMSE was in the moderate and high performance ranges in all cases for the monthly, crop phase, calendar season, and growing season, indicating good performance of the model for these periods. With the exception of snow depth and snowmelt for all averaging periods and of surface runoff during the growing season, PBIAS values showed that the model output had an insignificant bias. The averaging periods with most R² values in the moderate and high range were monthly, crop phase, crop year, calendar season, and growing season.

Nitrate leaching had an NRMSE indicative of high model performance (i.e., NRMSE < 50%) and minimal bias (0.8% < PBIAS < 7.8%) for all averaging periods. In addition, with the exception of the daily data comparison (R² = 0.28), the model output was highly correlated with the calibration data, with R² values ranging between 0.69 and 0.96. The model performance when the daily time interval is considered was low, despite the differences between averages for the calibration data and the model outputs being only 7.2%. This likely reflects the fact that the daily nitrate leaching values in the calibration dataset were estimated using concentration values measured approximately monthly. When the output was averaged on a monthly basis (Supplementary Material S7) and when all crop years were considered (i.e., “typical” averaging interval), all statistical indicators suggested a high model performance for nitrate leaching (i.e., NRMSE 19.9%, PBIAS −19.76%, R² = 0.65) (Supplementary Material S8). For this averaging interval, potatoes had the best fit for all statistical indicators (i.e., NRMSE 12.8%, PBIAS −2.88%, R² = 0.87). The barley and RC2 years had similar performance, with the exception of the NRMSE for RC2, which was significantly higher than for barley (i.e., 91.7% vs. 37.9%). The excellent fit for potatoes, which is the rotation phase with the highest contribution to nitrate leaching, is also supported by the minimal differences

between the model output and calibration data for this crop (i.e., $-3.6 \text{ kg NO}_3\text{-N ha}^{-1} \text{ yr}^{-1}$ for 2011 and $8.7 \text{ kg NO}_3\text{-N ha}^{-1} \text{ yr}^{-1}$ for 2014, with an average of $2.5 \text{ kg NO}_3\text{-N ha}^{-1} \text{ yr}^{-1}$). For the other crop phases, depending on the year, the RZWQM nitrate leaching output was either higher or lower than the nitrate leaching from the calibration data, with the model output being on average $5.6 \text{ kg NO}_3\text{-N ha}^{-1} \text{ yr}^{-1}$ lower than for the calibration data. Overall, for the period for which calibration data were available (2011–2016), the model underestimated nitrate leaching by $3.2 \text{ kg NO}_3\text{-N ha}^{-1} \text{ yr}^{-1}$.

Despite several months when the nitrate leaching from the model output was significantly different compared to the calibration data, the general trends and the magnitude of nitrate leaching were well reproduced by the model (Figure 3). The most significant periods where the model did not match the calibration data were in the summer of 2011 (potato), fall of 2012 (RC1), and from the mid-spring to mid-summer of 2014 (RC2 followed by potato) (Supplementary Material S9). These periods occurred during various times of the year and potato rotation phases and, hence, confirmed the unbiased performance of the model, as also evidenced by the PBIAS values.

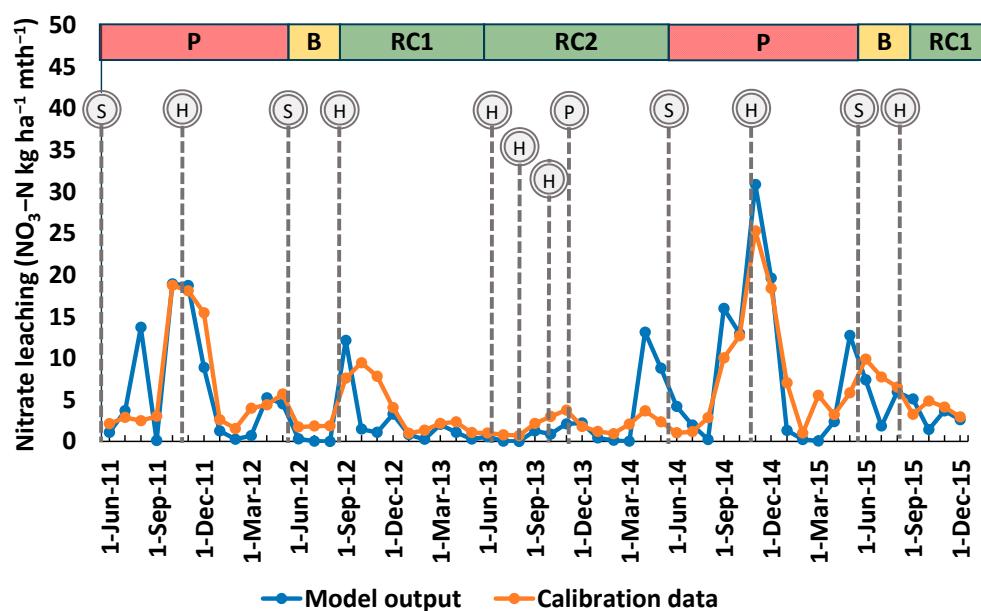


Figure 3. Monthly $\text{NO}_3\text{-N}$ leaching for Section A: model output vs. calibration data (S—seeding, H—harvesting, P—red clover plowed).

The comparison between the calibration data for sampling dates (i.e., discrete datasets), which included crop data and soil N amount, and the model output show that model fitness based on NRMSE and PBIAS for all parameters was high (Supplementary Material S10) when all crops were considered. This is confirmed by the generally small differences observed in averages of crop parameters for each sampling date (Supplementary Material S11). R^2 was also indicative of the high performance of the model for most parameters, with the exception of soil inorganic N and plant uptake (moderate performance) and plant uptake (low performance).

When considering the rotation phases separately, the potato had NRMSE values for almost all discrete datasets in the high model performance range (Supplementary Material S10). For potatoes, PBIAS had values smaller than 15.7% for all parameters, except for soil inorganic N and belowground biomass, thus suggesting minimal bias by the model. For potatoes, the model was able to predict fresh yield and dry tuber yield with high accuracy both during the growing season and at harvest time (Figure 4, Supplementary Materials S10 and S11). Other potato crop parameters measured in the field such as stolon dry weight, vine dry weight, and aboveground biomass were also indicative of the high fitness

of the model (Supplementary Material S11). Barley year (i.e., barley + RC1) averages had all indicators in the high model performance range. The aboveground dry weight, which was directly measured, confirms the high model performance for this crop phase during the entire growing season (Figure 4, Supplementary Materials S10 and S11). RC2 showed the lowest model performance when compared to the potato and barley rotation years. Thus, NRMSE values were in the low performance range for plant N accumulation (79.6%) in the high performance range for total biomass aboveground dry weight and in the moderate performance range for the other indicators. PBIAS for RC2 was in the moderate performance range for plant N uptake (52.6%) and soil N (42.9%) and in the high performance range for the other parameters. R^2 values were in the low performance range, despite several of the parameters showing a good match between the average of the measured and model output values (Supplementary Materials S10 and S11). The lack of fit for red clover could be potentially attributed to the incorrect recording of the cutting dates (Figure 4). Overall, the best model performance was achieved for potato and barley years, and the poorest performance for RC2.

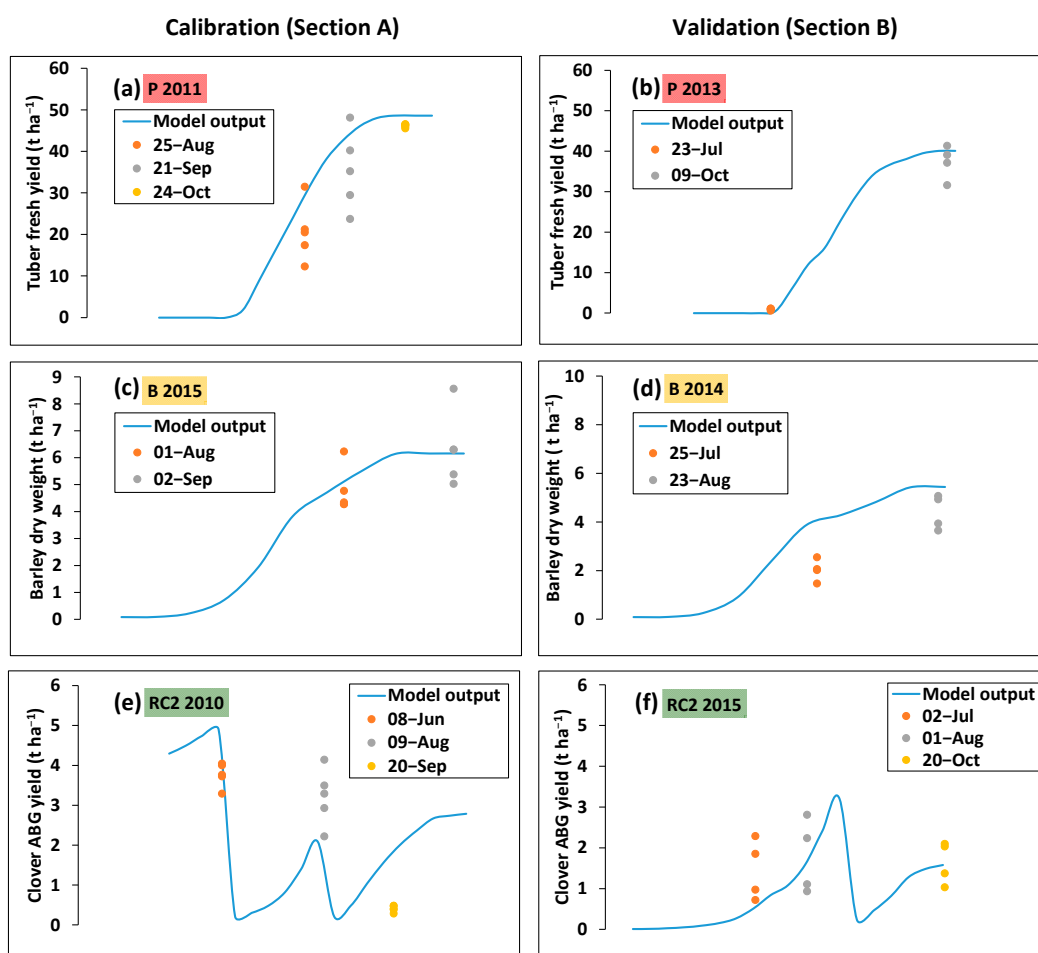


Figure 4. Comparisons between model output (lines) and measured data (dots) for selected crop parameters and years. (a) Potato (2011); (b) Potato (2013); (c) Barley (2015); (d) Barley (2014); (e) RC2 (2010); (f) RC2 (2015) (for barley, the biomass included total biomass for the first sampling date of the season and the sum of kernels and straw for the second sampling date of the season; ABG—aboveground biomass; for a given sampling date, each measured data dot represents a different location within the field).

The complete list of comparisons between the output of the calibrated model and the calibration data for various parameters is shown in Supplementary Material S8 for continuous datasets and in Supplementary Materials S10 and S11 for discrete datasets.

3.2. Model Validation

Nitrate leaching had an NRMSE and PBIAS indicative of high model performance (i.e., $\text{NRMSE} < 50\%$; $-17\% < \text{PBIAS} < 4.6\%$) for all averaging periods (Supplementary Material S12). R^2 suggested high model performance ($0.6 < R^2 < 0.9$) for all averaging periods except for the daily data comparison ($R^2 = 0.18$), despite the difference in average nitrate leaching between model output and validation data for the daily data being less than 1% (Supplementary Material S12). The nitrate leaching output from the validation simulation and the nitrate leaching estimated using the validation data are shown in Figure 5. As was the case with the calibration simulation, several months showed significant differences between the model output and the validation data (i.e., RC1 in October 2011, and potatoes between September and December 2013). For October 2011, the model overestimated the nitrate leaching by $11.4 \text{ kg NO}_3\text{-N ha}^{-1}$, resulting in an overall overestimation of nitrate leaching for the RC1 in 2011 of $7.3 \text{ kg NO}_3\text{-N ha}^{-1}$ (18.7%). For the fall of 2013, the model either overestimated (by up to $13.3 \text{ kg NO}_3\text{-N ha}^{-1}$) or underestimated (by up to $8 \text{ kg NO}_3\text{-N ha}^{-1}$) the nitrate leaching amounts from the validation dataset, thus resulting in much smaller relative differences for the respective potato year (i.e., $6.2 \text{ kg NO}_3\text{-N ha}^{-1}$ or 5.9%) when compared with the barley 2011 year. Overall, for the period for which validation data were available (2011–2016), the model underestimated the nitrate leaching from the validation data by $1.2 \text{ kg NO}_3\text{-N ha}^{-1} \text{ yr}^{-1}$, which is slightly smaller than the differences observed for the calibrated model (i.e., $3.2 \text{ kg NO}_3\text{-N ha}^{-1} \text{ yr}^{-1}$).

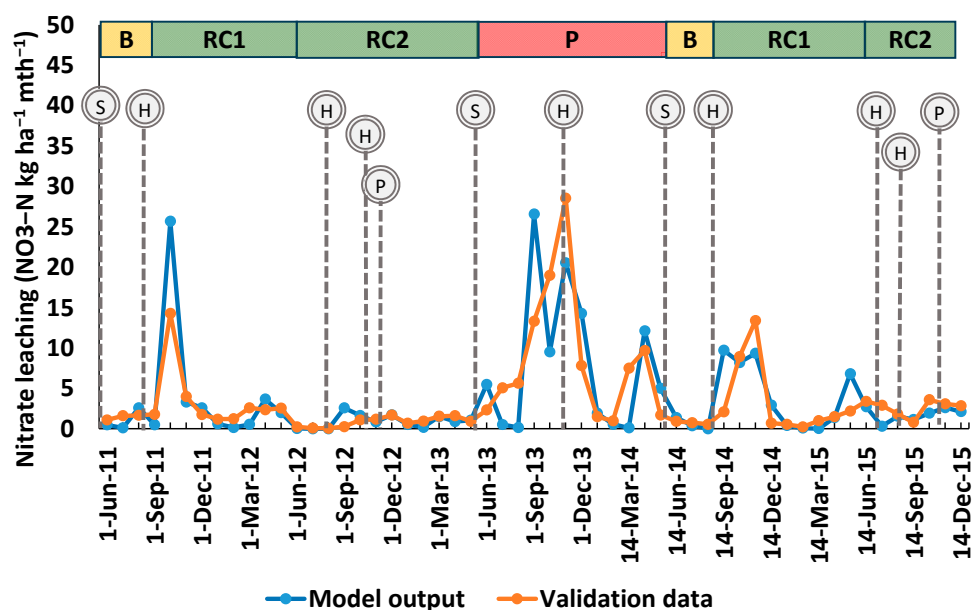


Figure 5. Monthly $\text{NO}_3\text{-N}$ leaching for Section B: model output vs. validation data (S—seeding, H—harvesting, P—red clover plowed).

Similar to the results of the calibration, the comparison between the validation data for sampling dates (i.e., discrete datasets) and the model output shows that model fitness based on NRMSE and PBIAS for all parameters was high (Supplementary Material S13) when all crops were considered. This is confirmed by the generally small differences observed in averages of crop parameters for each sampling date (Supplementary Material S14). R^2 was also indicative of the high performance of the model for most parameters, with the exception of belowground biomass (moderate performance) and total biomass (low performance). When considering the rotation phases separately, with the exception of belowground biomass (low performance), the potato had NRMSE and PBIAS indicative of high model performance (Supplementary Material S13). With no exception, the R^2 for all compared parameters was in the high performance range (i.e., $R^2 > 0.83$). Barley year

(i.e., barley + RC1) had NRMSE and PBIAS in the moderate or high model performance range, with the exception of belowground biomass, while R^2 had the belowground biomass and the plant N uptake in the low performance range. RC2 had NRMSE in the moderate or high performance range except for belowground biomass and plant N uptake; PBIAS for all parameters was in the moderate or high performance range. R^2 for RC2 was in the low performance range for all parameters, despite the averages of directly measured parameters (i.e., aboveground biomass) being close to the model output values, particularly towards the end of the growing season (Supplementary Material S14). Similar to the calibration simulation, the best model performance was achieved for potato and barley years, and the poorest performance for RC2.

The validation model fitness was similar to the one obtained for calibration, thus confirming that the model is suitable for simulating crop growth and nitrate leaching for the 3-year potato rotation implemented at the study site. The complete list of comparisons between the output of the validated model and the validation data for various parameters is shown in Supplementary Material S12 for continuous datasets and in Supplementary Materials S13 and S14 for discrete datasets.

3.3. Nitrate Leaching

Based on the calibrated model simulation, the largest cumulative soil N losses over a rotation cycle were from plant uptake (420 kg $\text{NO}_3\text{-N ha}^{-1}$) and nitrate leaching (148 kg $\text{NO}_3\text{-N ha}^{-1}$) (Table 3). Among the various rotation phases, the potato had both the highest plant uptake (171 kg $\text{NO}_3\text{-N ha}^{-1}$) and leaching (89.9 kg $\text{NO}_3\text{-N ha}^{-1}$). In our study, the leaching for the barley and RC2 years were comparable (28.6 kg $\text{NO}_3\text{-N ha}^{-1}$ and 29.7 kg $\text{NO}_3\text{-N ha}^{-1}$, respectively). Within the barley year, a quantity of 11.0 kg $\text{NO}_3\text{-N ha}^{-1}$ was leached under the barley and 17.6 kg $\text{NO}_3\text{-N ha}^{-1}$ under the RC1. In our study, when considering the length of each rotation phase (i.e., 100 days for barley, 268 for RC1, 367 days for RC2, and 363 for potato), the potato had the highest average daily leaching (i.e., 0.25 kg $\text{NO}_3\text{-N ha}^{-1}$), followed by barley (i.e., 0.11 kg $\text{NO}_3\text{-N ha}^{-1}$) and the clover phases (i.e., 0.066 kg $\text{NO}_3\text{-N ha}^{-1}$ for RC1, and 0.081 for RC2, respectively). Overall, 60.7% of the total leaching occurred during the potato year, 20% during the RC2 year, and 19.3% during the barley year (7.4% for barley and 11.9% for RC1). Previous nitrate leaching studies for PBC rotations under similar management in PEI provide a wide range of estimates [19,33,36,63]. Thus, estimates of leaching for potatoes varied between 80 and 215 kg $\text{NO}_3\text{-N ha}^{-1}$, for barley between 8.6 and 54 kg $\text{NO}_3\text{-N ha}^{-1}$, and for red clover between 35 and 172 kg $\text{NO}_3\text{-N ha}^{-1}$, with NH_4NO_3 inorganic fertilizer application rates varying between 150 and 200 kg N ha^{-1} for potatoes and 30 and 60 kg $\text{NO}_3\text{-N ha}^{-1}$ for barley, respectively. Jiang et al. (2011) [33], suggested that red clover, aside from being considered for its positive role in building the soil N supply for the potato crop, should also be considered in the nutrient management plans for its potential for significant leaching. In addition, Jiang et al. (2011) [33] recommended that the soil N reserve built during the red clover year be accounted for when estimating the required fertilizer amount for the potato phase.

Table 3. N budget terms for all crop phases (kg N ha^{-1}) *.

Crop Phase	N_{soil}	N_{fert}	N_{min}	N_{fix}	N_{upt}	N_{leach}	N_{oth}	Σ_{IN}	Σ_{OUT}	$\Sigma_{\text{IN}} - \Sigma_{\text{OUT}}$
Barley 2009	29.9	51.0	30.9	0.0	64.1	16.3	1.3	81.9	81.7	0.2
RC1 2009–2010	4.1	0.0	31.5	63.3	85.3	13.9	5.2	94.8	104	−9.6
Barley + RC1 2009–2010	11.5	51.0	62.4	63.3	149	30.1	6.5	177	186	−9.4
RC2 2010–2011	7.0	0.0	80.9	179	215	29.9	3.5	260	248	11.8
Potato 2011–2012	38.4	185	78.4	0.0	171	77.2	12	263	261	2.8
Barley 2012	42.3	51.0	18.4	0.0	65.4	0.4	2.1	69.4	67.8	1.6
RC1 2012–2013	7.4	0.0	39.9	12.2	39.3	22.4	4.6	52.1	66.3	−14.2
Barley + RC1 2012–2013	16.5	51.0	58.3	12.2	105	22.9	6.6	122	134	−12.6
RC2 2013–2014	9.7	0.0	88.8	14.8	63.3	29.7	2.9	104	95.8	7.8

Potato 2014–2015	53.4	207	84.5	0.0	172	103	15.9	291	290	1.2
Barley 2015	33.9	51.0	25.4	0.0	54.7	16.2	2	76.4	72.9	3.4
RC1 2015–2016	9.4	0.0	42.2	2.4	21.2	16.6	3.1	44.6	40.9	3.7
Barley + RC1 2015–2016	16.1	51.0	67.5	2.4	75.9	32.8	5.1	121	114	7.1
Averages for each crop										
Barley	26.8	51.0	24.9	0.0	61.4	11.0	1.8	75.9	74.2	1.8
RC1	7.2	0.0	37.8	26.0	48.6	17.6	4.2	63.8	70.5	−6.8
Barley + RC1	14.7	51.0	62.7	26.0	110	28.6	6	140	145	−5.0
RC2	8.3	0.0	84.4	96.7	138	29.7	3.1	181	171	10.0
Potato	45.7	196	81.4	0.0	171	89.9	14	277	275	2.0
Total for rotation	88.1	247	229	123	420	148	23.2	598	591	7.0

Notes: * RC1—Red clover 1, RC2—Red clover 2; N_{soil}—N in soil, N_{fert}—N from fertilizer, N_{min}—N mineralization, N_{fix}—N from fixation, N_{upt}—N plant uptake, N_{leach}—nitrate leaching; N_{oth}—Nitrate lost through other processes (i.e., surface runoff, immobilization, volatilization, denitrification, nitrous oxide emissions; Σ_{IN} —sum of N gains, Σ_{OUT} —sum of N losses.

The largest monthly leaching was estimated during the mid-fall to early winter of the potato phase (e.g., 30.9 kg NO₃-N ha⁻¹ in November 2014, 19.6 kg NO₃-N ha⁻¹ in December 2014, 18.9 kg NO₃-N ha⁻¹ in October 2011, and 18.7 kg NO₃-N ha⁻¹ in November 2011) (Supplementary Material S7). This is a period when plant uptake is much lower compared to the summer and early fall (e.g., the monthly average plant uptake for all crop phases was 8.1 kg NO₃-N ha⁻¹ in October compared to 29 kg NO₃-N ha⁻¹ in September), due to both a slowing down of plant metabolic processes and harvesting and is also a period that coincides with above-average precipitation amounts (e.g., 149.8 mm in October, 126.5 mm in November, and 163.5 mm in December compared to 108.8 mm monthly average for the entire year, when all rotation phases are considered) and reduced evapotranspiration (e.g., 42.6 mm in October, 30.9 mm in November, and 21.6 mm in December compared to 59.3 mm in September and 75.7 mm in August, when all rotation phases are considered). A period of secondary maximum monthly leaching was observed in mid- to late spring (i.e., April–May), a period corresponding to reduced plant uptake and increased drainage due to snowmelt.

The averages for each calendar season for the entire study period (Figure 6) show that 44% of the annual leaching occurred during the fall (i.e., 20.4 kg NO₃-N ha⁻¹), followed by spring (22.9% or 10.6 kg NO₃-N ha⁻¹), summer (18.5% or 8.5 kg NO₃-N ha⁻¹), and winter (14.6% or 6.7 kg NO₃-N ha⁻¹). For potatoes, most of the leaching occurred during the fall (54.3% or 48.8 kg NO₃-N ha⁻¹, followed by similar amounts for), with significant leaching continuing in the winter (17.6% or 15.8 kg NO₃-N ha⁻¹) and with the spring and summer showing the least nitrate leaching (14.3% or 12.8 kg NO₃-N ha⁻¹ and 13.9% or 12.5 kg NO₃-N ha⁻¹, respectively). For the barley year, most of the leaching occurred during the fall (38.6% or 11.0 kg NO₃-N ha⁻¹) and summer (36% or 10.3 kg NO₃-N ha⁻¹), with much less leaching occurring during the spring (14.5% or 4.2 kg NO₃-N ha⁻¹) and winter (10.9% or 3.1 kg NO₃-N ha⁻¹). For the clover year (i.e., RC2, most of the leaching occurred during the spring (62.9% or 18.7 kg NO₃-N ha⁻¹), followed by fall (19.8% or 5.9 kg NO₃-N ha⁻¹) and with much less leaching occurring during the winter (10.5% or 3.1 kg NO₃-N ha⁻¹) or summer (6.7% or 2.0 kg NO₃-N ha⁻¹). Overall, the leaching during the growing season, as determined by the average planting and harvesting dates for each crop, represented 62.3% of the annual leaching during the potato year, 71.8% during the barley year, and 18.1% during the RC2 year. The susceptibility of the fall and spring periods to nitrate leaching has also been confirmed in other studies conducted in PEI [63–65], highlighting that the majority of nitrate leaching can occur outside of the growing season.

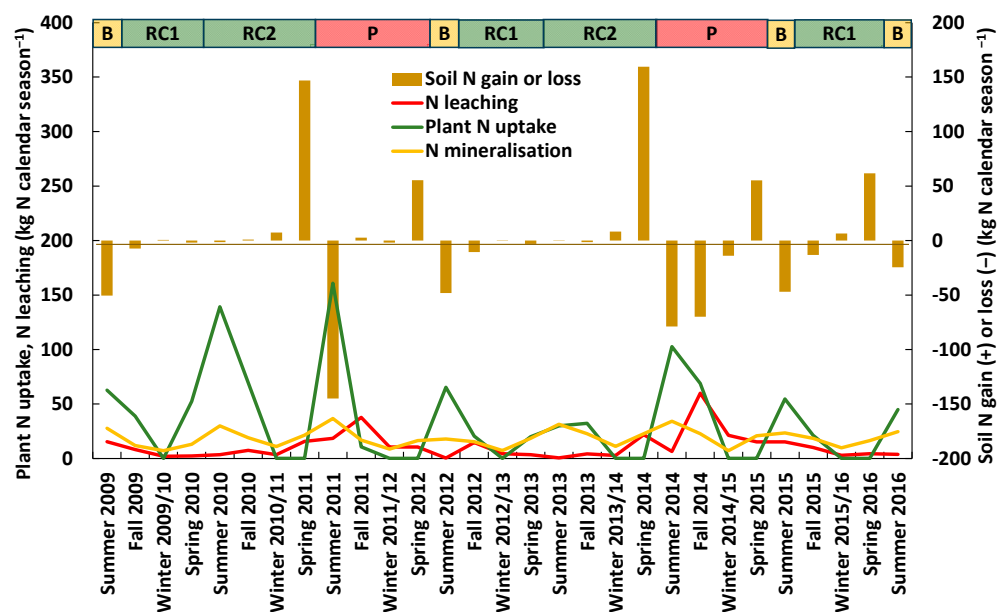


Figure 6. Calendar season averages of main soil N budget terms for the study period (2009–2016).

Compared to the total N inputs for each crop year, nitrate leaching represented 32.4% for potato, 20.5% for barley (14.5% for barley and 27.6% for RC1), and 16.4% for RC2. N use efficiency, defined using the methodology presented in Zebarth et al. (2004) [66], as the ratio between N supply via red clover accumulation (74.6 kg NO₃-N ha⁻¹ for RC1 and 236 kg NO₃-N ha⁻¹ for RC2) and fertilizer input (196 kg NO₃-N ha⁻¹ for potatoes and 51 kg NO₃-N ha⁻¹ for barley), and N removal via potato tuber (129 kg NO₃-N ha⁻¹) and cereal grain (39 kg NO₃-N ha⁻¹), was 30.2% for the entire rotation. If N accumulation in red clover was restricted to fixation only, the efficiency of the PBC rotation was 45.6%. The N use efficiency was very low as confirmed by other studies such as Jiang et al. 2022 [19], who found an efficiency of 33% for the PBC rotation. If only the potato year was considered, the N use efficiency was 69.4%, which is in the range of 60–80% efficiency found by Zebarth et al. (2004) [66] for the Russet Burbank potato variety; however, it should be noted that considering the efficiency for potato separately has the disadvantage of not considering the N supply provided by red clover to the potato crop and hence has limited value. The low N use efficiency suggests that implementing management practices such as the use of an alternative rotation phase or the introduction of more N-efficient potato varieties should be considered for improving N management for potato cropping systems.

The three-year PBC rotation is currently the PEI standard rotation [3,18,19], and the field management, soil, and climate conditions at HEF are also representative of most of PEI [3,18]. When extrapolating the results of the study to the PEI scale, where the percentage of land in potato rotation represents about 18.3% of PEI landmass [7], with about 6.1% of the land being planted with potatoes every year (i.e., three-year rotation), the nitrate leaching from the three-year potato crop rotation represents about 5112 t N ha⁻¹yr⁻¹, with 3099 t N ha⁻¹yr⁻¹ being attributed to leaching during the potato years. Estimates of N loading from potato production at the PEI scale are limited. Somers and Savard (2015) [67] estimated that ~8000 t N ha⁻¹ are leached annually to groundwater from agricultural sources. The respective study does not differentiate the load specifically sourced from potato cropping; however, it recognizes that potatoes are the dominant source. Grizzard et al. (2020) [13], based on land use data collected between 1996 and 2012 from 130 PEI watersheds, estimated that the annual nitrate load for the province was about ~6700 t N ha⁻¹yr⁻¹ and estimated that about 91% of the total nitrate load originated from agricultural areas.

Several previous studies have linked the intensive potato production systems to groundwater contamination in PEI [8–10] and also explored various BMPs for reducing

nitrate leaching [36,62,64]; however, a thorough review of these studies and their findings is required to support the development and implementation of targeted measures for reducing nitrate leaching by both policy regulators and farmers. In our study, the average leachate nitrate concentration in the calibrated model output for the complete rotation was 16.3 mg NO₃-N L⁻¹, while during the potato year, it averaged 34.9 mg NO₃-N L⁻¹, values which are above both the Canadian Maximum Acceptable Concentration (MAC) in drinking water of 10 mg NO₃-N L⁻¹ [68] and the Canadian nitrate in freshwater guideline for protection of aquatic life of 3.0 mg NO₃-N L⁻¹ [69], and hence they could be of concern for PEI, a province where groundwater quality is of critical importance as it provides the only source of drinking water and also is a significant contributor of nutrients to surface and coastal waters [10,70,71].

4. Conclusions

Extensive datasets collected between 2009 and 2016 from a field under a three-year potato–barley–clover (PBC) rotation located in Prince Edward Island (PEI), Canada, were used for calibrating and validating the soil water, N cycling, and crop components of a daily timestep model developed in RZWQM, with a particular focus on nitrate leaching and plant growth. To date, this is the first model developed in RZWQM for simulating potato rotation and the first PEI model to incorporate crop modelling for estimating nitrate leaching. The model calibration was complex, conducted via inverse modelling and trial and error, and involved 35 calibration datasets and adjusting of more than 150 parameters. The calibration procedure indicated a high or moderate model performance for most of the parameters tested using bivariate statistics (i.e., RMSE, NRMSE, PBIAS, R²) and for most of the averaging periods. The results of the model highlight that most of the nitrate leaching occurred during the potato year (89.9 kg NO₃-N ha⁻¹) and demonstrate that leaching during the red clover year (29.7 kg NO₃-N ha⁻¹) can exceed the leaching for the barley year (28.6 kg NO₃-N ha⁻¹). The model output also confirms that most of the nitrate leaching occurs outside of the growing season during fall and spring. The low N use efficiency for the PBC rotation (30.2% for the entire rotation), coupled with the presence of high nitrate concentrations in leachate for extended periods of time estimate and with the large extent of potato cropping systems in PEI, suggest that additional efforts need to be invested in optimizing both the composition and the management of the potato rotation systems in this area. The model developed in this study can be further used to support the adoption of measures aimed at reducing nitrate leaching and increasing the sustainability of agroecosystems for an industry-standard 3-year potato rotation under conditions typical of PEI. The model developed in this study can potentially support the development of additional models aimed at simulating intensive agricultural practices associated with potato cropping in other areas; however, further investigations would be necessary.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/w16030475/s1>, S1. Agricultural management for Field 355; S2. Datasets used for the calibration and validation of the RZWQM model; S3. SNOSWAB model calibration; S4. Values of RZWQM parameters after parametrization (P) and calibration (C); S5. RZWQM soil N budget equations; S6. Hydrograph separation using SepHydro; S7. RZWQM monthly soil N budget; S8. RZWQM Calibration: model output vs. continuous calibration datasets; S9. Nitrate leaching: periods with significant differences between the model output and the calibration dataset; S10. RZWQM Calibration: model output vs. discrete calibration datasets; S11. RZWQM Calibration: model output vs. crop data; S12. RZWQM Validation: model output vs. continuous validation datasets; S13. RZWQM Validation: model output vs. discrete validation datasets; S14. RZWQM Validation: model output vs. crop data; S15. Supplementary material references; Table S1. Description of the agricultural management operations for the potato–barley–red clover (PBC) rotation used in the study; Table S2. Datasets used for parametrization (P) and calibration (C) of the RZWQM model; Table S3. SNOSWAB Calibration results; Table S4. Values of RZWQM parameters following the parametrization (P) and calibration (C) of the model; Table S5. Monthly N budget terms for the calibrated simulation; Table S6. Comparison between model output for Section A and

continuous calibration datasets for various averaging intervals; Table S7. Comparison between model output for Section A and discrete calibration datasets for various averaging intervals; Table S8. Comparison between calibrated model output and measured crop growth parameters (Section A; discrete datasets); Table S9. RZWQM Validation: model output vs. continuous validation datasets; Table S10. Comparison between model output for Section B and discrete validation datasets for various averaging intervals; Table S11. Comparison between validation model output and measured crop growth parameters (Section B; discrete datasets) [72–88].

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Data Availability Statement: The data presented in this study are available on request from the corresponding author. SNOSWAB (Snow, Soil Water and Water Balance Model), SepHydro (hydrograph separation), ETCalc (evapotranspiration) and RECHARGE BUDDY (groundwater recharge) models used in this study are available at <https://www.hydrotools.tech> (accessed on 23 December 2023).

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