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Development of the DNDC model to improve soil hydrology and incorporate mechanistic tile drainage: A comparative analysis with RZWQM2

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ABSTRACT

The Denitrification Decomposition model (DNDC) has known limitations for simulating soil hydrology which can strongly influence biogeochemical processes. For this study, DNDC's soil hydrological framework was enhanced by including a new sub-model for mechanistic tile drainage, improved water flux, root growth dynamics, and a deeper and heterogeneous soil profile. Comparisons were then conducted against the Root Zone Water Quality Model (RZWQM2), using measurements of soil water storage, runoff, and drainage in eastern Canada and the US Midwest. Simulation of soil water storage (DNDC $0.81 \leq d \leq 0.90$; RZWQM2 $0.76 \leq d \leq 0.84$), daily water flow (DNDC $0.76 \leq d \leq 0.88$; RZWQM2 $0.77 \leq d \leq 0.90$) and nitrogen loading to tile drains were improved post-development. DNDC was able to capture the observed differences in water and N losses between conventional drainage and controlled drainage management with sub-irrigation. The enhancements to DNDC's hydrological framework should enable the development of improved biogeochemical processes.

1. Introduction

Efficient management of water and nutrients in agricultural systems is essential to further improve profitability for producers and to reduce greenhouse gases (GHG), losses of excess nitrogen (N), phosphorus and ammonia, which can contribute to global warming, eutrophication of water bodies and increases in atmospheric fine particulate matter. When considering the long-term sustainability of agriculture, it is of great importance to examine the interrelationships and trade-offs between crop productivity and all environmental outcomes.

There are numerous field and laboratory studies worldwide which focus on mitigating losses of nutrients, reducing GHG emissions and sequestering soil carbon in agricultural systems. However, due to extreme spatial and temporal variability in soils and climate, tools are required for extrapolating the knowledge gained from these studies over space and time. Because process based models, such as DayCent (del Grosso et al., 2001), the DeNitrification DeComposition model (DNDC; Li et al., 2012), the Root Zone Water Quality Model (RZWQM2; Ahuja et al., 2000) and APSIM (Thorburn et al., 2018), can dynamically simulate many of the interdependent process while maintaining a strict mass balance of nutrients and water, they are valuable for predicting N losses in the environment and assisting in the selection of best management practices (BMPs) (De Jong et al., 2009). While they offer valuable opportunities for expanding the scope of existing assessments, such models still have recognized knowledge gaps and thus require new targeted measurements for the development of improved mechanisms to ensure that the iterative process for model development continues. For instance, model structure is often limited by the oversimplified representation of soil and hydrological processes. In a review of nine GHG models, Brilli et al. (2017) found that 46% of the deficiencies in models were due to issues with the simulation of pedo-climatic conditions including soil-water simulation. In the same review DNDC was found to be the only model which simulated all C&N related GHG emissions considered. The DNDC model is the most prominent process-based model used for simulating GHG emissions worldwide, however, it has known issues in simulating soil hydrology (Smith et al., 2019; He et al., 2019, 2018; Brill et al., 2017; Congreves et al., 2016; Dutta et al., 2016a; Cui et al., 2014; Abdalla et al., 2011; Deng et al., 2011). These deficiencies impact the performance of the model for simulating C&N cycling and the timing of N_2O emissions (He et al., 2018; Uzoma et al.,

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2015; Smith et al., 2008). As a result, it has been suggested in many of these studies that DNDC development should be focused on improving the simulation of soil hydrology.

Several iterations of the DNDC model have been developed for different regions globally including New Zealand DNDC (Saggar et al., 2007), Landscape DNDC (Haas et al., 2013), China DNDC (Li et al., 2017) and Canada DNDC (Smith et al., 2013). Each one of these models can still be applied globally but they were developed to include additional processes and management options relevant to the locations where they were developed. In the case of the Canada DNDC model (DNDC.vCAN), it was designed to better simulate soil-plant–climate interactions in cool weather climate and has recently been improved for simulating evapotranspiration (Dutta et al., 2016a), ammonia volatilization (Dutta et al., 2016b; Congreves et al., 2016), impacts of snow cover and residue on soil temperature (Dutta et al., 2018), and improved growth of cool weather crops (He et al., 2019; Grant et al., 2016; Kroebel et al., 2011). Further, model developments from Canada DNDC were integrated back into the primary U.S. release version (Smith et al., 2019). However, as with any model, there remain shortcomings in the current model framework. Grant et al. (2016) identified that mineralization rates were too low in DNDC, sometimes resulting in excessive crop N stress. This can largely be attributed to the limitation that DNDC only simulates soil C&N processes over a 50 cm soil horizon. Also, in a detailed assessment of water processes in Canada DNDC, Smith et al. (2019) found that DNDC predicted crop biomass and monthly water and N flow to tile drains well but did poorly in predicting soil water content and daily tile flow events. In the same study, another model, RZWQM2, using more computational intensive hydrological processes, predicted good results but RZWQM2 requires more expertise to employ, greater simulation time, and is not well validated for simulating some biogeochemical processes. Since soil biogeochemical processes including chemical equilibria, nitrification, denitrification and fermentation are highly dependent on soil water content Smith et al. (2019) recommended the inclusion of a heterogeneous profile that exceeds crop rooting depths, root density functions, improved water flow and mechanistic tile drainage.

There is considerable complexity in developing improved soil structure, hydrology and tile drainage in DNDCv.CAN, while ensuring that the reliant biogeochemical mechanisms still function appropriately, but research has indicated that these improvements are critical towards the evolution of the model. An accurate estimate of soil hydrology is important for predicting the timing of N_2O emissions and N leaching events. Therefore, the objectives of this study were i) to improve DNDC for simulating soil hydrology, including the addition of a heterogeneous and deeper soil profile, root density functions, and improved water flow, ii) to incorporate a mechanistic tile drainage sub-model and include the ability to simulate a fluctuating water table, controlled drainage and sub-irrigation, and iii) to compare the performance of DNDC to the computationally intensive RZWQM2 using detailed datasets of runoff and drainage in eastern Canada and the US Midwest. It was deemed important that model developments be implemented at the minimum level of complexity and computation time necessary for improving accuracy, while keeping the user expertise at a manageable level.

2. Materials and methods

2.1. Description of experimental sites

2.1.1. Gilmore City, Iowa, USA experimental site

A five-year field experiment was established in the fall of 2004 and lasted until the end of 2009 at the Agricultural Drainage and Water Quality – Research and Demonstration Site close to Gilmore City in north central Iowa, USA. The site soils are predominantly characterized as Nicollet (fine-loamy, mixed, superactive Aquic Hapludoll), Webster (fine-loamy, mesic Typic Endoaquolls), Canisteo (fine-loamy, mesic Typic Endoaquolls), and Okoboji (Fine, smectitic, mesic Cumulic Vertic Endoaquolls). General site characteristic are shown in Table 1 and detailed soils data by horizon are presented in Table S1. Four land cover treatments were initiated with the first two consisting of alternating phases of winter rye cover crop prior to maize or prior to soybean (first phase of the rotation TileDrain-CoverCrop-MaizeSoybean [TD-CC-MS] and second phase of the rotation TileDrain-CoverCrop-SoybeanMaize [TD-CC-SM]). The next two treatments were alternating phases of maize and soybean with no cover crop (first phase of rotation TileDrain-NoCoverCrop-MaizeSoybean [TD-NCC-MS] and second phase of rotation TileDrain-NoCoverCrop-SoybeanMaize [TD-NCC-SM]) (Table 2). Aqueous ammonium nitrogen was applied to maize at a rate of 140 kg N ha^{-1} in the spring near emergence time. The site includes a large compliment of measurements including water content across 4 depths, crop yields, biomass and daily measurement of water flow and N concentration to tile drains. See Qi et al. (2011a, b) for a more detailed description of soil, management and experimental setup.

2.1.2. Woodslee, Ontario, Canada experimental site

A study was conducted at the Honorable Eugene F. Whalen Experimental Farm, Woodslee, Ontario Canada (42°13′N, 82°44′W) to monitor surface runoff and tile drainage (Drury et al., 2014). The Brookston clay-loam soil at the site is classified as an Orthic Humic Gleysol (Canadian Classification system) or a poorly drained, fine, loamy, mixed, mesic, Typic Argiaquoll in the USDA system (Tables 1 and S1). The study was of 5 years duration starting in late 1999 and ending in early 2005 (Table 3). Treatments included a maize-soybean rotation and unrestricted tile drainage with (TD-CC-MS) and without (TD-NCC-MS) a winter wheat cover crop and also controlled drainage and sub-irrigation with (CDS-CC-MS) and without (CDS-NCC-MS) a cover crop. This data helped to facilitate testing the new controlled drainage/sub-irrigation feature in DNDC. Both a starter (18-46-0) and sidedress application of UAN (150 kg N ha^{-1}) was applied to maize for a combined nitrogen rate of 175 kg N ha^{-1}. Maize grain was harvested in early November and tillage generally consisted of fall disking except when excessive residue required a more substantial cultivated heavy plow. Two flow meters were used in each plot to measure cumulative surface runoff and drainage flow. Samples of surface water and runoff were collected using an autosampler every 500–3000 L of flow and analysed for NO_3^- concentration. From June to July 2001 intact soil cores were collected for determination of bulk density, saturated hydraulic conductivity and soil water retention at 9 matric potentials. See Drury et al. (2014) for a more detailed description of soil, management and experimental setup.

2.2. Model description

2.2.1. DNDC model

The DNDC model was developed originally to simulate N_2O emissions (Li et al., 1992) and gained popularity due to its detailed biochemical equations describing nitrification and denitrification processes. It was later expanded to simulate soil C&N cycling, water and N movement (Li et al., 2006) and full farm nutrient cycling (Li et al., 2012) and now contains sub-models for simulating crop biomass, decomposition, nitrification denitrification, fermentation and ammonia volatilization. The model simulates a very wide array of agricultural management and crop types, the input requirements are reasonable and it can be applied with relative ease. As a result, DNDC has been used extensively worldwide (Ehrhardt et al., 2018; Brilli et al., 2017; Zhang and Niu, 2016; Gilhespy et al., 2014; Giltrap et al., 2010). Many users have, however, reported that the model had issues in simulating soil water content (Smith et al., 2008, 2019; He et al., 2018; Brilli et al., 2017; Congreves et al., 2016; Dutta et al., 2016a; Uzoma et al., 2015; Cui et al., 2014; Abdalla et al., 2011; Deng et al., 2011) which is correlated with soil oxygen content, a driver for the growth and death of nitrifier and denitrifier bacteria in DNDC. Since soil water content impacts the type and rate of microbial reactions in DNDC it can greatly impact N_2O emissions. Furthermore, since DNDC only simulates soil C&N cycling to

Table 1
Site characteristics at Gilmore City and Woodslee research plots.

Location and data collection period	Soil classification[a]	Average annual temp.	Average annual precip.	Average growing season precip.	Soil characteristics			
					Soil surface texture	Soil Organic Carbon	pH	Bulk density
		(oC)	(mm)	(mm)	(%)	(g kg^{-1})		(g cm^{-3})
Woodslee, Ontario, Canada 42°13′N, 82°44′W (1999–2005)	Poorly drained, fine, loamy, mixed, mesic, Typic Argiaquoll	9.8	816	491	28 sand 35 silt 37 clay	25.0	7.0	1.42
Gilmore City, Iowa, United States 42°42′N 104°00′W (2005–2009)	Nicollet (fine-loamy, mixed, superactive, mesic Aquic Hapludoll)	8.7	824	578	33 sand 35 silt 32 clay	23.2	7.1	1.34

[a] Other soil series are also present at the Gilmore City site.

a 50 cm depth, processes such as nitrification, denitrification, nitrate leaching, fermentation, ammonium fixation, and mineralization may be represented inaccurately to account for the limited depth of simulation.

DNDC employs a simple layered cascade approach for simulating bulk water flux and N transport down the soil profile. Water drains to field capacity in each layer (~2 cm thickness) at the rate of K_{SAT} (Fig. 1). Both water flow and C&N cycling are simulated to 50 cm depth through a homogeneous soil profile. A deep water pool, with a water holding capacity based on its bulk density, is situated below the 50 cm soil profile to provide water for crop transpiration (50 cm soil profile + 50 cm deep water pool = 100 cm total water pool). The model rooting depth is fixed with transpiration being drawn equally across all soil layers, followed by extraction from the deep water pool when plants are under water stress. To improve the simulation of water and N loss to tiles Li et al. (2006) incorporated a simple "recession curve" to delay drainage by soil layer but this is not active in the current U.S. DNDC release version. Smith et al. (2019) tested this approach and although the simulated drainage was improved soil water content was then overestimated by 22% and N_2O emissions increased by 26%.

Since 2011 a Canadian version of DNDC (now referred to as DNDCv.CAN) has been under development to improve the simulation of agricultural management and crop cultivars in cool weather climate. Smith et al. (2019) compared DNDCv.CAN to RZWQM2 and found limitations in its ability to simulate soil hydrology thus suggested several improvements including a deeper and heterogeneous soil profile, improved water flow down the profile, root density functions, a fluctuating water table and mechanistic tile drainage. In this study we incorporate these developments while attempting to minimize extra model inputs, complexity for users and computation time. In this study Canada DNDC prior to development is referred to as "default DNDC" and Canada DNDC post development is referred to as "revised DNDC".

2.2.2. RZWQM2

RZWQM2 (version 3.0.2015; Ahuja et al., 2000; Ma et al., 2012) was developed to simulate detailed biogeochemical processes in cropping systems with a major focus on simulating water quality. The model simulates a wide array of agricultural management and has recently been expanded and improved for simulating N_2O emissions (Fang et al., 2015; Jiang et al., 2019) and phosphorous dynamics (Sadhukhan et al., 2019). RZWQM2 includes DSSAT 4.0 crop models with CERES and CROPGRO components (Hoogenboom et al., 2017; Ma et al., 2005, 2006) which is a very well established framework for simulating crop growth and development worldwide. RZWQM2 uses a numerical solution to determine water fluxes and includes the Green-Ampt equation for infiltration, the Richards equation with an option for lateral hydraulic gradient for lateral water loss, and the Hooghoudt's equation for simulating quasi-2D tile drainage. Thus the model input requirements, modeller expertise and computation time are greater than for DNDC. The model has been validated for simulating drainage and N loading to tiles at many locations in North America (Malone et al., 2017; Xian et al., 2017; Qi et al., 2011b; Li et al., 2008; Thorp et al., 2007; Akhand et al., 2003) and has been employed to investigate BMPs for reducing N losses. Since RZWQM2 is a well-recognized model for simulating soil hydrology it offers an excellent opportunity for benchmarking DNDC developments.

Table 2
Cropping systems and agronomic practices at the Gilmore City site, Iowa from 2005 to 2009 (adapted from Smith et al., 2019). Treatment abbreviations are as follows: TD, unrestricted tile drainage; CC, cover crop; NCC, no cover crop; MS, maize-soybean; SM, Soybean-maize.

	2005	2006	2007	2008	2009
Treatment					
TD-CC-MS, Calibration	rye-maize	rye-soy.	rye-maize	rye-soy.	rye-maize
TD-NCC-MS, Validation	maize	soybean	maize	soybean	maize
TD-CC-SM, Validation	rye-soy.	rye-maize	rye-soy.	rye-maize	rye-soy.
TD-NCC-SM, Validation	soybean	maize	soybean	maize	soybean
Management activity					
Termination of rye prior to maize	April 30	April 24	April 30	May 6	May 8
Cultivation[a] and maize planting	May 10	May 4	May 14	May 15	May 19
Cultivation[a] and soybean planting[b]	May 18	May 10	May 17	May 23	May 20
Termination of rye	May 20	May 16	May 23	May 26	May 31
Maize fertilizer (@140 kg N ha^{-1})	May 25	May 18	June 5	June 4	June 30
Maize and soybean harvest	Oct. 10	Oct. 7	Oct. 22	Oct. 20	Nov. 3
Chisel plow (NCC rotations)	Oct. 10	Oct. 10	Oct. 24	Oct. 20	no-till (wet)
Disk plow and cultivation (CC rotations)	Oct. 10	Oct. 10	Oct. 24	Oct. 20	no-till (wet)
Plant rye	Oct. 11	Oct. 12	Oct. 25	Oct. 21	Nov. 20

[a] Only TD-NCC-MS and TD-NCC-SM were cultivated.
[b] DNDC handles intercropping but not RZQWM2, thus for RTWQM2 soybean was planted after rye termination.

Table 3
Cropping systems and agronomic practices at the Woodslee site, from 2000 to 2005. Treatment abbreviations are as follows: TD, unrestricted tile drainage; CDS, controlled drainage with sub-irrigation; CC, cover crop; NCC, no cover crop; MS, maize-soybean.

	2000	2001	2002	2003	2004	2005
Treatment						
TD-CC-MS, Calibration	ww-maize	ww-soy.	ww-maize	ww-soy.	ww-maize	ww-soy.
TD-NCC-MS, Validation	maize	soybean	maize	soybean	maize	soybean
CDS-CC-MS, Validation	ww-maize	ww-soy.	ww-maize	ww-soy.	ww-maize	ww-soy.
CDS-NCC-MS, Validation	maize	soybean	maize	soybean	maize	soybean
Management activity						
Termination of ww[a]	May 8	May 23	May 21	May 27	June 3	May 19
Plant soybeans		June 8		June 17		May 31
Plant maize and starter (25 kg N ha^{-1})	May 17		May 22		June 4	
Sidedress (UAN at 150 kg N ha^{-1})	June 22		June 18		June 22	
Soybean harvest		Nov 6		Oct 6		Oct 26
Maize harvest	Nov 8		Nov 4		Nov 10	
Fall disking	Nov 8	Nov 6	Nov 6	Nov 6	Nov 22	
Plant winter wheat	Nov 8	Nov 7	Nov 7	Nov 7	Nov 23	

ww – winter wheat.
[a] Roundup (1.4 kg ha^{-1} a.i.) was used to terminate ww in 2000, 2003, and 2004 whereas Vantage (1.4 kg ha^{-1} a.i.) was used in 2001 and 2002. All plots were sprayed.

2.3. Development of DNDC to improve the simulation of soil hydrology and to include mechanistic tile drainage

2.3.1. Heterogeneous and deeper soil profile

The default DNDC model only characterizes the top soil horizon and assumes a homogeneous profile throughout. Often this is not a good representation of agricultural soils which can have striking differences across depths as a result of changing textures and organic carbon contents. Therefore, the model interface was restructured to allow for the user input of soil properties by definable layer depths. Soil properties that are now defined by depth include bulk density, soil organic carbon, pH, soil texture, field capacity, wilting point, porosity and saturated hydraulic conductivity. The user can specify the depth of the soil profile up to 200 cm and define properties for up to 10 user defined depths. The soil profile information can be saved such that it can be used for other simulations.

The modifications to the model interface were conducted in parallel with the model simulation depth being adjusted from 50 cm to 200 cm (Fig. 1). The total number of simulated layers were increased to ensure that the calculated layer thickness remained in the same range (~0.5–2.5 cm) as it was previously for the 50 cm version of the model. This was important since many processes are formulated to calculate the mass and energy flows based on this conceptual range of layer thickness. It was decided that 200 cm would provide a sufficient depth to accommodate the effective root penetration of most commonly used crops and allow for the simulation of a fluctuating water table and tile drainage. Modifications to internal variables were conducted to ensure that soil properties, water, carbon, nutrients, and temperature could be tracked over the entire depth and these variables could be applied for estimating decomposition, denitrification, nitrification, fermentation, adsorption onto clay, chemical equilibria and N movement functions. As a result, DNDC was not only enhanced for simulating soil hydrology but also for

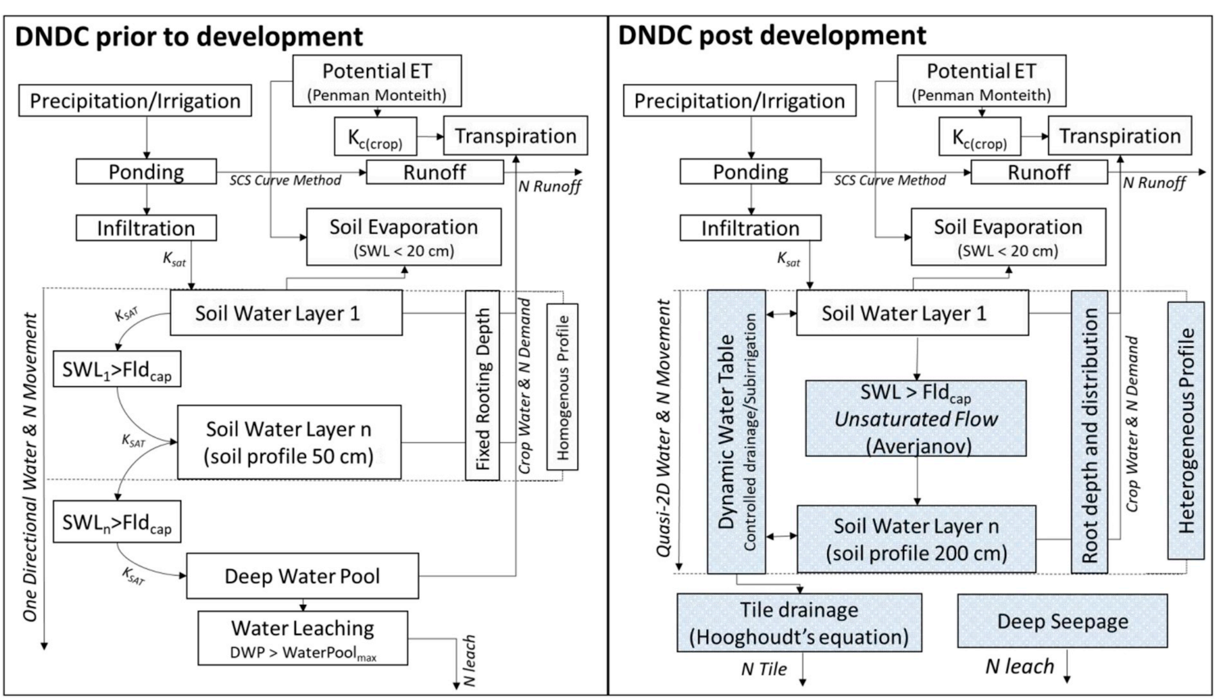

Fig. 1. Schematic of Canada DNDC before and after development of improved hydrological processes. Shaded areas show which algorithms were modified. Revised model version available at https://github.com/BrianBGrant/DNDCv.CAN.

the simulation of all biogeochemical processes up to a 200 cm depth.

2.3.2. Root penetration and density function

The default DNDC model calculates a linear estimate of root penetration to a maximum depth of only 50 cm, without considering root density. Since water uptake for transpiration is partitioned equally across the profile, this can result in the model underestimating water and N uptake near the surface and overestimating these components in the deeper profile. Further, crops only have access to 100 cm of soil water when the deep water pool is included (Fig. 1), thus deeper rooted crops can sometimes become water limited. As a result of these limitations in the default model, a root penetration equation based on growing degree days (GDD) (Pedersen et al., 2010) was incorporated into DNDC. Temperature or GDD are considered to be the main drivers for root growth and penetration (Kage et al., 2000; Thorup-Kristensen, 2006; Kirkegaard and Lilley, 2007). The equation, expressed in terms of PGI (Plant Growth Index) which is the fraction of accumulated degree days required for a plant to reach maturity in DNDC is as follows;

$$R_z = \begin{cases} R_{zmin}; & PGI \le PGI_{lag} \\ \sum\left(\left(PGI - PGI_{lag}\right)k_{rz}\right) + R_{zmin}; & PGI > PGI_{lag} \\ R_{zmax}; & PGI - PGI_{lag}k_{rz} + R_{zmin} > R_{zmax} \end{cases} \tag{1}$$

where R_z is the depth of root penetration; R_{zmin} is the planting depth; PGI_{lag} accounts for the time period between planting and start of root penetration (germination); k_{rz} is the root depth penetration rate with values provided for some crops in Pedersen et al. (2010); R_{zmax} is the maximum root penetration depth. The R_{zmax} value is user defined in the DNDC input interface.

An algorithm for root distribution, based on a study by Gerwitz and Page (1974), and further modified by Yang et al. (2009) to extend the rooting depth of fine roots by an additional 30% was also employed in DNDC. The root density declines logarithmically to the root penetration depth (R_z) followed by a linear decrease to zero at $1.3R_z$. The relative root length distribution is as follows;

$$L_R(z) = \begin{cases} e^{-a_z z}; & z < R_z \\ e^{-a_z z}\left(1 - \dfrac{z - R_z}{0.3R_z}\right); & R_z \le z \le 1.3R_z \end{cases} \tag{2}$$

where a_z is the shape parameter describing root distribution with increasing soil depth. Pedersen et al. (2010) used values of $a_z = 2$ for wheat and winter wheat and 1.5 for brassica's and we currently use a default value of 2 but the user can define the shape parameter and rooting depth based on field studies or from sources such as Fan et al. (2016) and Benjamin et al. (2013).

2.3.3. Simulating water flow

The default cascade flow algorithm, whereby water content per layer tips to field capacity on an hourly basis can result in an erroneously low prediction of soil water contents. Complex numerical schemes, such as finite difference and finite element solutions of Richard's equation, can generally produce more accurate result; however, they are data and computation intensive. It is possible to use pedotransfer functions to estimate water retention curves and other hydrological parameters for use in these equations but in doing so it can undermine much of the improved accuracy that is achieved using this approach. Further, there is some uncertainty regarding the applicably of Richards equation for highly heterogeneous agricultural soils. In a review of water flow approaches, Beven and Germann (2013) commented that in unsaturated heterogeneous soils there is rarely a consistent hydraulic gradient, which Richard's equation assumes, since capillary potentials are not in equilibrium.

Initially, we investigated including an integrated-Richards-equation approach with the van Genuchten equation (van Genuchten, 1980) for estimating soil water retention characteristics in DNDC, as presented in Yang et al. (2009) but once implemented, the hydrology sub-model time step needed to be reduced to such an extent that the computational time of DNDC was greatly increased and we also found it difficult to obtain data to properly fit the van Genuchten or other water retention equations. During the course of development, after the inclusion of a heterogeneous soil profile, root density function and mechanistic tile drainage, we found that the cascade approach could provide sufficient accuracy in estimating water contents/flux. We decided to keep the cascade flow approach intact but limited water movement above field capacity based on soil water status using the following simple approach derived by both Averkjanov (1950) and Irmay (1954) for estimating unsaturated conductivity.

$$K = K_{SAT}\left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^n \tag{3}$$

where K is hydraulic conductivity, K_{SAT} is saturated hydraulic conductivity, θ is actual, θ_r residual, and θ_s saturated soil water content (cm^3 cm^{-3}). This equation differs in power (n) where Irmay used a value of 3 and Averkjanov 3.5. Our tests indicate that a value of 3.5 worked well in the range of soil water contents from field capacity to saturation, the only incidence when K is calculated in revised DNDC.

2.3.4. Fluctuating water table

DNDC was modified to simulate a fluctuating water table by adjusting the hydraulic conductivity of the deepest profile to near impermeable (user defined value). A water table slowly builds up from the bottom soil layer with deep seepage at the lower boundary. The water table is maintained as a mass balance of incoming water from precipitation and irrigation and outgoing water from runoff, evapotranspiration, tile drainage, deep seepage and change in soil water content in unsaturated layers. For the purposes of estimating tile flow rate, the water table height was calculated at the top of the saturated soil layer closest to the soil surface.

2.3.5. Incorporating a tile drainage sub-model

Similar to RZWQM2 and DRAINMOD (Skaggs et al., 2012), the steady state Hooghoudt equation was also included in DNDC. The drawdown of water table height is not fully steady state, however, the rate of change usually proceeds slow enough that the Hooghoudt equation can be used effectively (Skaggs et al., 2012). A recent study by Xian et al. (2017), when assessing the performance of RZWQM2 using the original steady state equation and two transient equations, found that there was no significant difference in model performance for hourly drainage simulation. The Hooghoudt equation as written in Skaggs et al. (2012) is;

$$q = \frac{4K_e m(2d_e + m)}{L^2} \tag{4}$$

where q ($cm\ h^{-1}$) is the drainage discharge rate, K_e ($cm\ h^{-1}$) is the effective lateral hydraulic conductivity, m is the water table level above the drain at midpoint between the drains, d_e is the equivalent depth to the impermeable (or restrictive) layer below the drain, and L is the drain spacing. Equations to estimate K_e and d_e below were outlined in Xian et al. (2017).

$$K_e = \frac{\int_{i=1}^{i=n} D_i K_i}{\int_{i=1}^{i=n} D_i} \tag{5}$$

where n is the number of soil layers, D_i is the thickness of layer i (cm), and K_i is the lateral hydraulic conductivity of layer i ($cm\ h^{-1}$).

As indicated in Xian et al. (2017) the calculation of d_e depends on the actual depth (d) of the soil profile:

$$\text{if } \frac{d}{L} < 0.3 \quad d_e = \frac{d}{1 + \frac{d}{L}\left[\left(\frac{8}{\pi} ln \frac{d}{r}\right) - CON\right]} \tag{6}$$

where

$$CON = 3.55 - 1.6\frac{d}{L} + 2\left(\frac{d}{L}\right)^2 \tag{7}$$

$$\text{if } \frac{d}{L} \geq 0.3 \quad d_e = \frac{L}{\left(\frac{8}{\pi} ln \frac{L}{r}\right) - 1.15} \tag{8}$$

where r is the radius of the drain (m).

2.3.6. Movement of nitrogen to runoff, tile drains and through the soil profile

The primary development aim of this study was to improve estimation of soil hydrology and thus the existing N movement mechanisms in DNDC were not extensively modified. The default nitrate movement in DNDC is described simply as a function of the water flux and nitrate concentration per layer. Soil nitrate was considered to be mobilized by a positive water flux (90% mobilized) and transferred to the layer below as a one-dimensional vertical N flux towards the bottom soil profile. Additionally, another fraction (10% of the NO_3^- in a layer) was considered to be lost through preferential water flow via macropores directly out of the soil profile. This preferential loss was calculated regardless of whether the soil layer directly below also met the condition of having a positive water flux.

For simulations now with tile drainage, the movement of nitrate is an iterative step through each of the saturated layers per hour that are drained to tiles. In DNDCv.CAN this preferential N leaching function was modified to ensure correlation with water movement. It was previously found that DNDC sometimes simulated N losses when there was no water flux out of the bottom of the soil profile. In DNDCv.CAN the fraction of NO_3^- available to be transferred to the layer below at an hourly time step can now be parameterized through the user interface with a default value of 0.9. The fraction per layer that is preferentially lost directly to drains (i.e. it bypasses the iterative layer loop) is set to a default fraction of 0.02. Nitrate losses to tile drains are calculated starting from the layer situated at the top of the saturated water table down to the layer at the bottom of the tile drains.

Additionally, we found that in default DNDC nitrate losses to runoff were always very low, irrespective of the soil conditions, water inputs or crop management employed. To address this issue we first fixed a water mass balance error in the SCS runoff curve number method. Second, the model was modified to simulate a fluctuating water table and when the water table reaches the soil surface runoff and additional loss of N could then occur. Further, N loss to runoff was originally calculated as a fraction of rainfall that goes to runoff (based on SCS method) multiplied by the nitrate found in only the top surface layer (~0.5–2 cm). We extended this calculation to the top 2 layers (~1–4 cm) and included a user defined parameter where the fraction can be adjusted.

2.4. Initialization, calibration and validation

At both the Gilmore city and Woodslee research locations the TD-CC-MS treatment was used for model calibration and the remaining 3 treatments were used for validation. A similar trial and error method for calibration as conducted in Smith et al. (2019) was used where the RMSE for simulated yield, drainage and N loss to tiles was minimized. This was conducted for default DNDC, revised DNDC and RZWQM2. In all simulations, a 10 year spin-up was included prior to the experimental periods to stabilize soil C, N and water.

Experimental data from the sites was used to initialize the models. This data included soil properties, such as soil texture, bulk density, field capacity, wilting point, porosity, saturated hydraulic conductivity and soil organic carbon content (Table S1). Note that soil data was only available at two depths at the Woodslee site, thus the properties from the 10–20 cm depth were extrapolated down to 200 cm. Daily weather data, including min and max temperature, precipitation, wind speed, solar radiation and relative humidity, were available at both sites for all years of the studies. Management data, including tillage scheduling and implements and fertilizer scheduling and application rates, was also available.

For the Gilmore City site, default DNDC and RZWQM2 have previously been calibrated and validated (Smith et al., 2019). In this study we compare the performance of the revised DNDC model to those results. After the hydrology developments had been implemented, the revised model was calibrated using the same approach as the other two models. Crop, soil and tile drainage parameters used in the study for default and revised DNDC are shown in Table S2 and crop parameters used in RZWQM2 are shown in Table S3. Note that a winter rye cultivar was not available in RZWQM2, thus Qi et al. (2011b) developed parameters based on a winter wheat cultivar and these were further modified for a more recent version of RZWQM2 by Smith et al. (2019).

2.4.1. Calibration of crop parameters in DNDC

For revised DNDC, several crop parameters were calibrated however parameters remained close to those used by default DNDC. The thermal degree days to maturity (TDD) was increased marginally for both maize and soybean (Table S2). Water requirement for maize and soybean were reduced. At Gilmore city, soybean was set to 340 g water per g dry matter which is very close to the default 350 value for the U.S. release version. In default DNDC plant roots only had access to the top 100 cm of the profile and had no access to a water table which was a structural deficiency. The crop water requirements needed to be increased in the default model to simulate an appropriate level of crop water uptake, evapotranspiration and drainage which often resulted in soil water content that was too low in the growing season (Smith et al., 2019). In the revised model appropriate rooting depth and uptake from a fluctuating water table was simulated thus crops were less water stressed and crop water requirements were calibrated to be on average 15% lower for maize and 23% lower for soybean.

At the Woodslee location the average soybean yields were only 60% of that at Gilmore City. We believe this was partly due to different varieties being used than at Gilmore City (a different variety was planted every year at Woodlsee as the soybean variety A2553 was no longer available in 2005 and a shorter-season variety was planted in 2003 as a result of a late plant date: Drury et al., 2014). We used a lower maximum grain C parameter (optimum yield) at Woodslee for soybean (Table 2). However, the main contributing factor was likely that more crop water stress occurred at Woodslee. This was attributed to greater runoff due to a lower permeability soil and more precipitation occurring in the off-season months. Also, Woodslee receives less average precipitation on average, during the growing season than at Gilmore City (Fig. S1).

In default DNDC, rooting depth is always constant at 50 cm. In revised DNDC we set a lower max root depth at Woodslee site (0.8 m for maize and 1.1 m for soybean) since there is higher clay content and lower root penetration (Table S2). This helped minimize RMSE for yields and drainage. Rooting depth in DNDC was set considerably lower than in RZWQM2 which has max possible root depth of 1.8 m for both maize and soybean.

For the winter-rye cover crop at Gilmore City, the parameters used in Smith et al. (2019) for default DNDC were employed for revised DNDC. Default parameters for both default and revised DNDC were used for the winter wheat cover crop grown at the Woodslee site. The winter rye and winter wheat cover crop never reached the grain filling stage before being terminated in any of the treatments simulated. A similar magnitude of winter wheat biomass was simulated for DNDC and RZWQM2 at Woodslee but no measured data was available for validation.

2.4.2. Calibration of soil and drainage parameters in DNDC

The drainage development required the integration of additional input parameters to the DNDC interface including drain depth, spacing and radius, depth to bedrock, and K_{SAT} at each depth. Lateral K_{SAT} is estimated as 2*K_{SAT} (Qi et al., 2011b) which is needed to calculate K_e for use in the Hooghoudt equation. In general, it is very difficult to get a good measure of in situ K_{SAT}, particularly at deeper soil depths. Laboratory measurements of K_{SAT} using soil cores and the traditional saturated flow-desorption method can in fact be over an order of magnitude greater than in situ measured K_{SAT} (Smith et al., 1995). In this study we used the K_{SAT} values from Qi et al. (2011b) for the Gilmore City site and adjusted K_{SAT} with depth for the Woodslee site to values that would provide a good estimate of tile drainage using both DNDC and RZWQM2 (Table S1).

During the calibration process for default DNDC, it was necessary to reduce the size of the slow humus soil organic carbon (SOC) pool from a default value of 0.95 to 0.7 to provide sufficient N mineralization when simulating the observed levels of N losses at the Gilmore City site (Smith et al., 2019). Using revised DNDC it was only necessary to reduce this parameter to 0.90. The revised DNDC model simulates decomposition to 200 cm and thus it estimates a more plausible rate of mineralization, which was previously noted to be a model weakness in some studies (Grant et al., 2016; Smith et al., 2008). Similar to the Gilmore City location, for default DNDC it was necessary to reduce the size of the slow humus SOC pool in default DNDC from 0.95 to 0.75 to simulate the correct magnitude of N losses in the calibration treatment at Woodslee. Using revised DNDC this value was decreased only to 0.91. The SCS curves number for estimating runoff in revised DNDC at Gilmore city was set to 64, the same value as used for default DNDC (Smith et al., 2019). A value of 87 was used at Woodslee for both model versions to account for a lower permeability soil and thus simulate the correct level of runoff for the calibration treatment. Preferential movement of N was set to 2% in revised DNDC to allow rapid movement of a small portion of N to drains, without moving through the soil matrix. This improved the model performance at both sites.

The N concentration in precipitation was set to 1.8 mg N L^{-1}, the same value as used at the Gilmore City site (Qi et al., 2011b). The microbial parameters related to nitrification and denitrification rates were left as default, however, during the course of development we added several new parameters into the DNDC input interface such that they could potentially be adjusted. The rate of microbial activity can vary greatly between soil types and locations.

2.4.3. Calibration of RZWQM2 at Woodslee site

A similar procedure employed in Smith et al. (2019) and Qi et al. (2011b) at the Gilmore City site was used for calibrating RZWQM2 at the Woodslee site. Measured soil properties were input into the model according to Table S1. Initial soil moisture was set to saturation below the 60 cm depth at the beginning of the 10 year spin-up to initiate the simulation of a water table. The magnitude of the initial soil carbon was based on site measurements, however, the partitioning of the SOC pools was determined by using a built in tool for equilibrating SOC based on total SOC at the soil surface, global position and regional temperatures. Similar to Smith et al. (2019) at the Gilmore City site it was necessary to increase the decomposition rate of the SOC pools by about 30% at the Woodslee site in order to simulate the appropriate level of N mineralization and subsequent N losses to tile drainage and runoff. The simulated organic N levels in the soil profile remained stable over the five year study. The N concentration in precipitation was set to the same total N input rate as for DNDC with values of 0.5 mg N L^{-1} and 1.3 mg N L^{-1} for NH_4^+, and NO_3^- respectively.

The impermeable layer was set at 390 cm with a K_{SAT} rate of 0.01 cm h^{-1} in the bottom layer which limited flow and maintained a water table. The Brookes-Corey soil water retention model was used with curve fitting parameters being estimated internally in RZWQM2 based on measured water contents at saturation, 1/10 bar, 1/3 bar and 15 bar (wilting point).

Similar to DNDC, the crop parameters in RZWQM2 needed to be lowered to simulate the appropriate level of crop yields at the Woodslee location, particularly for soybean. A number of the DSSAT crop parameters for maize (IB 1068 Dekalb 521) and soybean (990002 M Group 2) were left as default, particularly the ones controlling phenology, however, to optimize RMSE for biomass for the calibration treatment at Woodslee we reduced three crop parameters for maize and five parameters for soybean (Table S3). Default parameters for winter wheat (990003 winter-US) were used at Woodslee.

2.5. Statistical measures for testing model performance

Model performance of default DNDC, revised DNDC and RZWQM2 were evaluated using several statistical measures including normalized average relative error (NARE; %), normalized root mean square error (NRMSE; %), Nash-Sutcliffe model efficiency coefficient (NSE; Nash and Sutcliffe, 1970) and the d index (Wilmott and Matsuura, 2005).

$$NARE = 100\left(\frac{\frac{1}{n}\sum_{i=1}^{n}\left(P_i - O_i\right)}{\overline{O}}\right) \tag{9}$$

$$NRMSE = 100\left(\frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(O_i - P_i\right)^2}}{\overline{O}}\right) \tag{10}$$

$$NSE = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \overline{O})^2} \tag{11}$$

$$\mathrm{d} = 1 - \frac{\sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(|P_i - \overline{O}| + |O_i - \overline{O}|)^2} \tag{12}$$

where P_i is the predicted or simulated value and O_i is the observed value.

NARE is the average percent over- or under-prediction of a model relative to measurements. Both NRMSE and NARE are commonly used to evaluate model performance for estimating yield and biomass. Jamieson et al. (1991) indicated that a model had excellent performance if NRSME < 10; good < 20; fair < 30; and poor > 30 whereas Ahuja et al. (2000) indicated satisfactory performance if NARE < 15% for estimating yield and biomass.

NSE and d statistics are commonly employed for estimating water and N leaching and runoff. An NSE value of greater than 0 indicates the model estimates are more accurate than the average of observations. NSE has a maximum value of 1 and a negative NSE indicates poor model performance. However, NSE is more sensitive to values that have higher deviation (Kraus et al., 2005) and may in certain instances be close to zero or negative even when model results are very close to measurements (but the measurements show little deviation), thus it is important to also assess ARE and RMSE. The d index provides a qualitative assessment of model accuracy with $d \geq 0.9$ showing an “excellent” agreement between model and observed values, $0.8 \leq d \leq 0.9$ indicates a “good” agreement, $0.7 \leq d \leq 0.8$ a “fair” agreement and $d < 0.7$ a “poor” agreement. For water drainage and N flow to tiles Moriasi et al. (2007) considered model performance to be satisfactory if NSE > 0.5. Drainage was satisfactory if NARE <25% and N loss to tiles if NARE <70%.

Table 4
Statistical performance of models for simulation crop yields at Gilmore City and Woodslee.

Treatment	Crop	Default[a] DNDCv.CAN			Revised DNDCv.CAN			RZWQM2[a]		
		NARE	RMSE	NRMSE	NARE	RMSE	NRMSE	NARE	RMSE	NRMSE
		(kg DM ha^{-1})			(kg DM ha^{-1})			(kg DM ha^{-1})		
Gilmore City										
TD-CC-MS[b]	Maize	7.3	1028	12.8	4.8	1284	16.0	0.4	1337	16.7
TD-NCC-MS	Maize	1.7	962	11.4	0.6	1133	13.4	−4.0	1184	14.0
TD-CC-SM	Maize	−4.6	852	9.6	2.3	679	7.7	0.9	236	2.7
TD-NCC-SM	Maize	−8.7	818	8.9	−5.7	559	6.1	1.7	509	5.5
TD-CC-MS[b]	Soybean	0.2	171	5.9	−0.9	215	7.4	2.2	63	2.2
TD-NCC-MS	Soybean	−8.9	377	12.0	−8.8	382	12.1	−5.5	181	5.8
TD-CC-SM	Soybean	13.7	575	22.3	13.4	586	22.8	14.0	538	20.9
TD-NCC-SM	Soybean	10.1	425	16.0	8.8	376	14.2	12.1	348	12.1
Woodslee										
TD-CC-MS[b]	Maize	2.6	1152	15.9	−6.7	694	9.6	0.8	978	13.5
TD-NCC-MS	Maize	2.0	798	10.8	−7.2	778	10.5	−4.8	735	10.0
CDS-CC-MS	Maize	NA	NA	NA	11.4	834	11.6	5.5	597	8.3
CDS-NCC-MS	Maize	NA	NA	NA	13.4	974	13.8	7.5	781	11.1
TD-CC-MS[b]	Soybean	−2.0	328	17.3	−4.9	156	8.2	−1.1	330	17.4
TD-NCC-MS	Soybean	1.0	280	15.9	3.1	127	7.2	7.1	339	19.3
CDS-CC-MS	Soybean	NA	NA	NA	17.0	421	21.8	4.9	420	21.7
CDS-NCC-MS	Soybean	NA	NA	NA	38.5	675	40.1	41.7	767	45.6

[a] Simulations for default Canada DNDC and RZWQM2 at Gilmore City site were performed by Smith et al. (2019).
[b] Calibration treatment.

3. Results and discussion

It was previously demonstrated that the default version of Canada DNDC performed well for simulating crop yields, monthly water and N loss to tile drains at the Gilmore City (Smith et al., 2019). In this study we verified that the revised model performed well for these components, however, most of the emphasis was placed on testing the model for simulating soil water storage and daily N and water loss to tile drains at Gilmore City, for which it did not previously perform well and also for simulating drainage and runoff at the Woodslee site. In addition we tested the new functionality of the model for simulating controlled drainage and sub-irrigation.

3.1. Simulation of crop yields

The revised DNDC model performed well in simulating crop yields at the Gilmore City site (Table 4) giving similar results as both the previously tested models, default DNDC and RZWQM2, as reported by Smith et al. (2019). All three models demonstrated good to excellent performance (NRMSE < 20%) for yield estimates except for soybeans in the TD-CC-SM treatment which were over-predicted in 2007 and 2009. These were years which had lower seasonal GDD, perhaps supressing observed yields. The models were only calibrated in 2006 and 2008 (Table 2) thus they may have under-predicted this impact. It was interesting that the improvements to hydrology simulation, as will be demonstrated in subsequent sections, did not improve yield prediction for this site with average statistic being similarly good between models. The RMSE levels in this study were generally lower than those in Jerecki et al. (2018) where the estimates for maize were over 1100 kg DM ha^{-1} using DNDC.vCan.

At the Woodslee location, all models demonstrated good to excellent performance (NRMSE's < 20%) for simulating maize and soybean yields under the unrestricted tile drainage calibration and validation treatments (Table 4). Note that revised DNDC performed better than default DNDC for maize and large improvements were observed for soybean likely as a result of the improved hydrology simulation. Crops are generally more water limited at Woodslee due to more off-season runoff and less growing season precipitation. Maize yields were also well simulated by both revised DNDC and RZWQM2 for both the CC and NCC treatments under CDS. Of course, default DNDC was not capable of simulating controlled drainage or sub-irrigation. Both DNDC and RZWQM2 showed fair performance in simulating soybean yield under CDS-CC but interestingly their performance was poor for CDS-NCC with about a 40% overestimation of yields. Revised DNDC produced similar NRMSE values as RZWQM2, demonstrating the value of running more than one model for a study. Both models simulated less crop water stress in this system with controlled drainage and sub-irrigation. In investigating measurements, the CDS-NCC system appears to have behaved counterintuitive to what might have been expected since observed overall runoff + drainage to tiles was about 10% less than the other 3 treatments (Table S4), yet crop yields (and assumedly evapotranspiration) were similar. One explanation is that there may have been more deep seepage for this plot which is further discussed in subsequent sections.

3.2. Soil water storage at Gilmore City

As demonstrated by Smith et al. (2019) soil water storage was poorly simulated by default DNDC and reasonably simulated by RZWQM2. This was the case across all four treatments. Some of the main issues were that DNDC did not include root density functions, a heterogeneous profile or unsaturated flow. During this development, we found that characterizing these aspects improved the model, particularly the addition of root density functions. Higher root density near the soil surface resulted in more water uptake near the soil surface (Fig. 2; 0–6 cm depth) thereby improving the water content simulation. However, the largest improvement for simulating soil water content resulted from the inclusion of a fluctuating water table and mechanistic tile drainage. Default DNDC greatly under predicted soil water storage at deeper depths in the summer months primarily because crop roots had no access to the water table. Post-development, the roots could now penetrate beyond 50 cm to a depth defined by the user, with fine roots penetrating 30% further, and potentially allowing plant roots to access the water table. This greatly improved the model fit for simulating soil water content at deeper depths (Fig. 2) and soil water storage to 60 cm depth (Fig. 3). As demonstrated by the statistical performance (NSE and

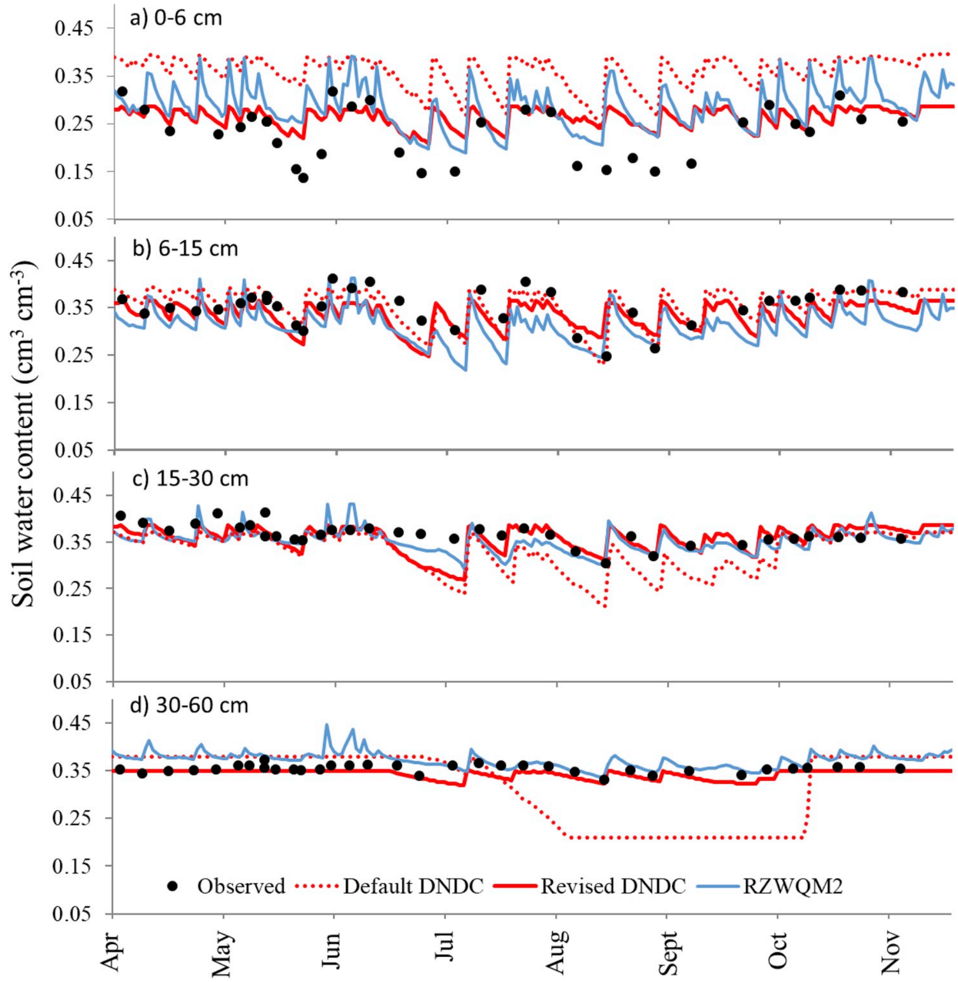

Fig. 2. Observed and simulated soil water content by depth in 2008 for validation treatment TD-CC-SM at Gilmore City.

d) of default and revised DNDC (Table 5) soil water storage was improved for all treatments from fair/poor ($0.69 \leq d \leq 0.79$) performance to good/excellent ($0.81 \leq d \leq 0.90$) performance. All three models predicted the average magnitude of soil water content well during the 5 year study ($-1.3 \leq \text{NARE} \leq 4.6$), however, revised DNDC and RZWQM2 performed much better in predicting the trends over time. Revised DNDC had similar performance as RZWQM2 for the CC treatments and had improved performance for the NCC treatments. Interestingly, the soil water storage as predicted by RZWQM2 indicated that drainage from the profile was sometimes more delayed in relation to observations. This may be related to an issue with using Richard's equation since it assumes a consistent hydraulic gradient which often does not exist in heterogeneous agricultural soils (Beven and Germann, 2013).

3.3. Tile drainage at Gilmore City

The implementation of a water table, mechanistic tile drainage and root penetration functions in DNDC resulted in the simulation of a fluctuating water table that was distinctly similar to RZWQM2 (Fig. S2). A similar level of water table draw down during the growing season occurred each year, due to crop water uptake (transpiration) and also the rise in water table after rainfall events and the time required for drainage to the tile depth were similar. As a result the simulated daily water flow to tile drains was often remarkably similar as is demonstrated in validation treatment TD-CC-SM (Fig. 4). The daily predicted drainage flows for revised DNDC and RZWQM2 often overlapped. We found that the inclusion of Hooghoudt's equation was particularly crucial for simulating the correct timing of events, which gave DNDC the same functionality of commonly used water quality models such as RZWQM2 and DRAINMOD (Skaggs et al., 2012). Default DNDC, which simulates bulk flux of water down the profile via the cascade approach, simulated peak flow events that were too high and diminished too quickly, however, monthly flow was well simulated (Table 5).

Revised DNDC demonstrated excellent performance ($d \geq 0.90$; $\text{NSE} \geq 0.69$) for simulating monthly water flow to tile drains for the three validation treatments, with marginal improvements over default DNDC, which was previously found to perform well for monthly flow (Smith et al., 2019) (Table 5). All three models predicted the correct average magnitude of drainage from TD-CC-MS and TD-NCC-MS treatments but under-predicted the drainage from treatment TD-CC-SM and over-predicted it from TD-NCC-SM. Observations indicated that more loss occurred to tile drains from TD-CC-SM (with cover crop; 347 mm over 5 years) than TD-NCC-SM (without cover crop; 252 mm over 5 years) which is unexpected. This disparity may be attributed to measurement variability during peak flow events in 2007 and 2008 which were high (Smith et al., 2019). This variability was not taken into account in the model performance statistics. All three models predicted more transpiration and less water loss to tile drains in treatments with cover crops than without. Experimental studies generally report no difference in subsurface drainage (Drury et al., 2014; Qi et al., 2011a, 2011c; Kaspar et al., 2007) or reduced drainage (Qi and Helmers, 2010; Strock et al., 2004) when a cover crop was present. The performance of revised DNDC for simulating daily drainage was improved in all

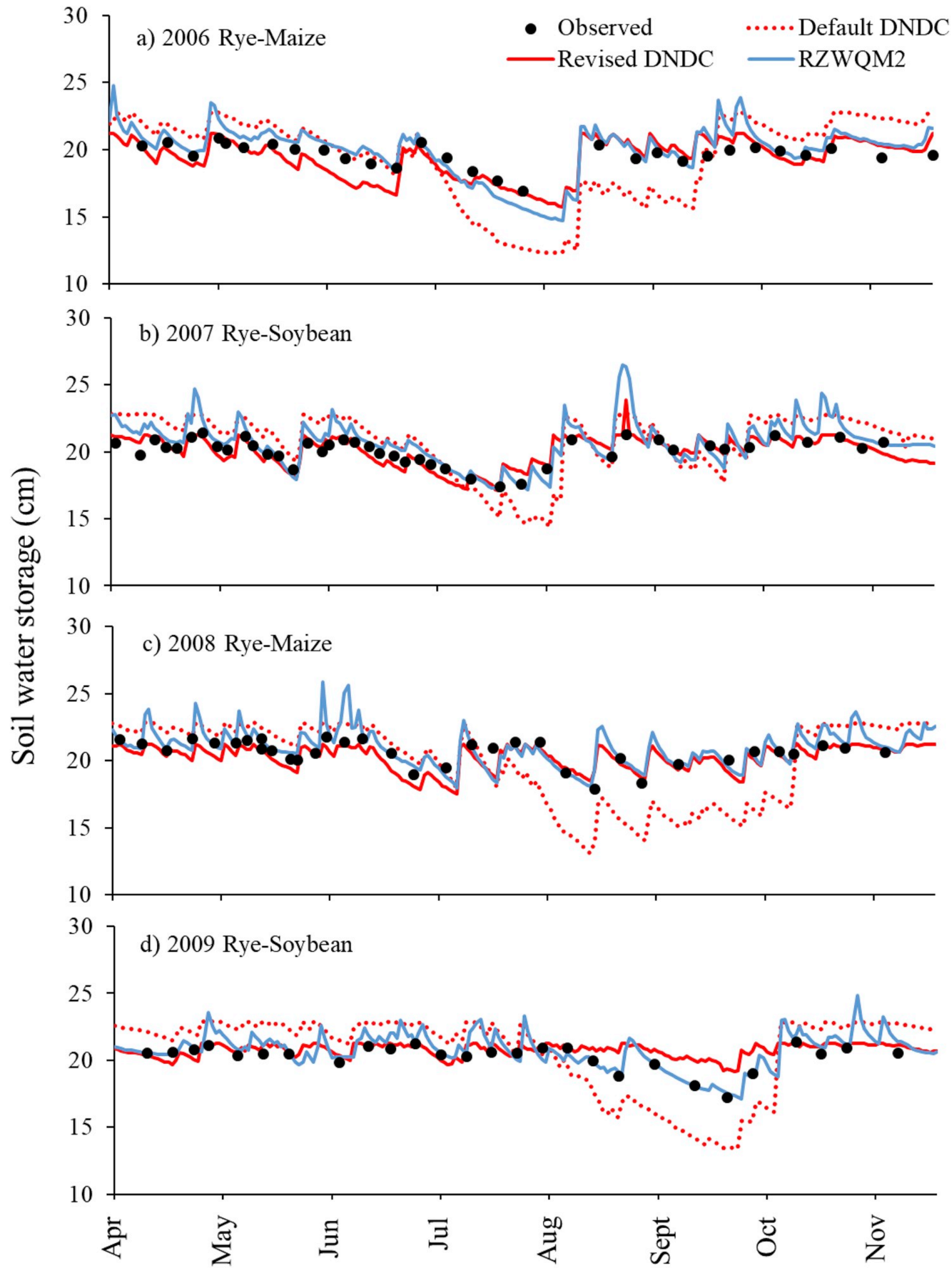

Fig. 3. Observed and simulated soil water storage to 60 cm depth for validation treatment TD-CC-SM at Gilmore City.

treatments, particularly for TD-CC-MS and TD-NCC-SM where NSE values went from negative (worse than the average of measurements) to > 0.5 (Table 5). Note that daily measurements were only available in 2007 and 2008 (Qi et al., 2011b). The d statistic indicated that simulations changed from being characterized as poor to fair (i.e. d from 0.68 to 0.74) to fair to good (i.e. 0.76 to 0.88). Average statistics across treatments were similar between revised DNDC and RZWQM2 indicating that developments were successfully implemented. In particular, we found that the inclusion of mechanistic tile drainage improved the performance of revised DNDC, which is consistent with David et al. (2009) who found that models designed to simulate tile drainage (SWAT, EPIC and Drainmod-N), performed better for simulating bulk water flux than those which did not (DayCent, DNDCv.82a and DNDCv.82h). Malone et al. (2017) compared the performance of the HERMES model to RZWQM2 for simulating water and N loss to tile drains. The HERMES model, which did not include mechanistic drainage, performed reasonably well but RZWQM2 performed better in simulating monthly drainage. Guest et al. (2017) found that Canada DNDC performed similarly to DayCent and STICS models for simulating soil water dynamics, but the three models all included cascade water flux approaches at the time. In a cross-Canada assessment Guest et al. (2018) found that Canada DNDC performed a little better than the water budget models VSMB and HOLOS, but the water budget models did not explicitly simulate crop water stress and the feedbacks from crop growth and development.

The revised DNDC improved the simulation of monthly N loss to tile drains, demonstrating excellent performance across all treatments, with better NSE and d statistics than both default DNDC and RZWQM2. Note that N concentrations in tile drainage were measured less frequently than water volumes (Qi et al., 2011b). Similar to water flow, all 3 models under-predicted N loss for the TD-CC-SM treatment and over-predicted for the TD-NCC-SM treatment. However, similar to the models, most

Table 5
Statistical performance of models for simulating drainage and N loss to tile drains at the Gilmore City research site.

Water/N component	Statistic	Calibration			Validation								
		TD-CC-MS[a]			TD-NCC-MS			TD-CC-SM			TD-NCC-SM		
		Default DNDC	Revised DNDC	RZWQM2	Default DNDC	Revised DNDC	RZWQM2	Default DNDC	Revised DNDC	RZWQM2	Default DNDC	Revised DNDC	RZWQM2
Soil water storage (0–60 cm depth)	NARE	1.9	−1.3	1.1	4.6	1.7	4.3	0.8	−0.6	1.9	2.8	1.1	4.5
	NSE	−1.05	0.41	0.46	−4.52	0.11	−0.52	−3.61	0.35	0.08	−1.18	0.46	−0.03
	d	0.79	0.88	0.87	0.69	0.81	0.76	0.72	0.84	0.84	0.74	0.90	0.77
Tile drainage (monthly, 2005–2009)	NARE	1.6	3.9	6.0	−5.3	−0.8	−1.4	−16.1	−15.2	−13.3	17.5	16.0	24.5
	NSE	0.73	0.69	0.67	0.71	0.74	0.76	0.65	0.72	0.65	0.62	0.72	0.60
	d	0.92	0.90	0.90	0.91	0.92	0.92	0.87	0.90	0.87	0.90	0.93	0.90
Tile drainage (daily, 2007–2008)	NARE	−2.6	−6.9	3.2	−10.3	−13.7	−9.2	−22.9	−20.2	−18.5	8.2	3.1	14.5
	NSE	−0.32	0.55	0.35	0.08	0.51	0.50	0.24	0.60	0.50	−0.11	0.70	0.69
	d	0.68	0.80	0.76	0.71	0.76	0.79	0.74	0.81	0.77	0.67	0.88	0.90
N loss to tiles (monthly, 2005–2009)	NARE	7.4	8.9	0.2	−3.0	−4.6	−1.4	−10.7	−3.1	−17.8	14.1	11.7	13.7
	NSE	0.53	0.69	0.67	0.65	0.77	0.67	0.59	0.75	0.51	0.58	0.64	0.44
	d	0.85	0.92	0.89	0.89	0.93	0.91	0.83	0.93	0.82	0.86	0.92	0.86

[a] TD – unrestricted tile drainage; CDS – controlled drainage and subsurface irrigation; CC – cover crop; NCC – No cover crop; MS - Maize-soybean rotation phase; SM – Soybean-maize rotation phase.

studies show reduced N loss to tiles when a cover crop was included (Malone et al., 2017; Drury et al., 2014; Li et al., 2008; Kaspar et al., 2007; Parkin et al., 2006; Strock et al., 2004). At the Gilmore city site the difference in N loss between the treatments, based on observations, was not found to be significant (Qi et al., 2011a) and thus the higher average annual loss from TD-CC-SM (39.9 kg ha^{-1} y^{-1}) relative to TD-NCC-SM (33.7 kg ha^{-1} y^{-1}) may be related to measurement variability.

Most of the development in this study focused on improving soil hydrology and drainage, however, we still found it necessary to adjust the way N moved and was simulated in DNDC (both U.S. DNDC and DNDCv.CAN). The model was adjusted to simulate N loss to tiles at the depth of the drains, but also to only allow preferential N movement to occur when there was water movement. This improved the timing of simulated N loss events, as is demonstrated for validation treatment TD-NCC-MS in Fig. 5. Although the simulated upper soil profile was frozen and there was no water movement in the fall and winter of 2005, N loss to tiles was still simulated using default DNDC. Simulating preferential N movement as a function of water flow, the implementation of N loss to drains at the specified depth, and improved simulation of hydrology were responsible for the improved statistics noted in Table 5.

3.4. Impacts of hydrology developments on GHG emissions at Gilmour City

Although measurements of N_2O or CH_4 emissions were not available at this site, the impact of the hydrology developments was substantial. For the revised model simulated N_2O emissions were reduced by 41% on average across the 5 years with an example shown in Fig. S3 for the validation treatment TD-CC-SM where emissions were reduced by 34%. The reduced emissions were primarily caused by increased crop water uptake near the soil surface, resulting in much lower soil water contents (Fig. 2). In DNDC, nitrification and denitrification reactions occur primarily near the soil surface where substrates are high, thus emissions were strongly impacted and reduced by the lower soil water content simulation in the surface 15 cm. More emissions were simulated in the spring after snowmelt in revised DNDC primarily because inorganic soil N was higher. There was 11.1 kg ha^{-1} less simulated N loss to tiles during the winter period for revised DNDC relative to default DNDC because preferential N movement was prevented from occurring when there was no water flux.

Note that in default DNDC water "tips" to field capacity on an hourly basis, however, it is known that N_2O production should occur above field capacity, usually at about 80% WFPS (Butterbach-Bahl et al., 2013). The improvement of the hydrology framework will allow for future research whereby the denitrification reactions can be set to occur in the proper ranges of soil water and oxygen contents. Water content is also a driver of N_2O diffusion and N_2O production and consumption which can also now be targeted for improvement.

The soil at Gilmour City has good drainage and is well aerated thus there was no simulated production of CH_4 from methanogenisis for either model version, however, simulated CH_4 uptake by oxidation increased from 0.38 to 0.628 kg C ha^{-1}y^{-1} on average across the five year study for the revised model relative to the default model.

3.5. Runoff and tile drainage at Woodslee

Although soil water contents were not available at the Woodslee site, there was an opportunity to benchmark the simulation of water and N loss to runoff along with the implementation of controlled drainage and sub-irrigation for DNDC. In general, the revised DNDC model demonstrated "good" to "excellent" performance ($0.83 \leq d \leq 0.96$; Table 6; Fig. 6) for simulating tile drainage for the validation treatments, with notable improvement over default DNDC ($d \leq 0.68$; "poor" performance) for the unrestricted tile drainage treatments. Default DNDC does not have the capability of simulating controlled drainage or sub-irrigation and thus could not be evaluated for these aspects. RZWQM2

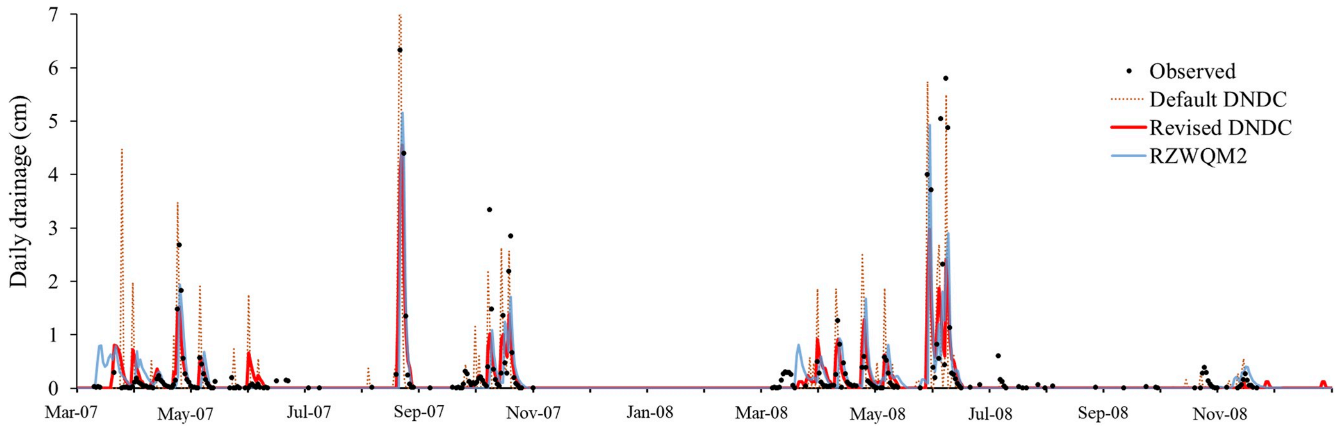

Fig. 4. Observed and simulated daily water flow to tile drains for validation treatment TD-CC-SM at Gilmore City from 2007 to 2008.

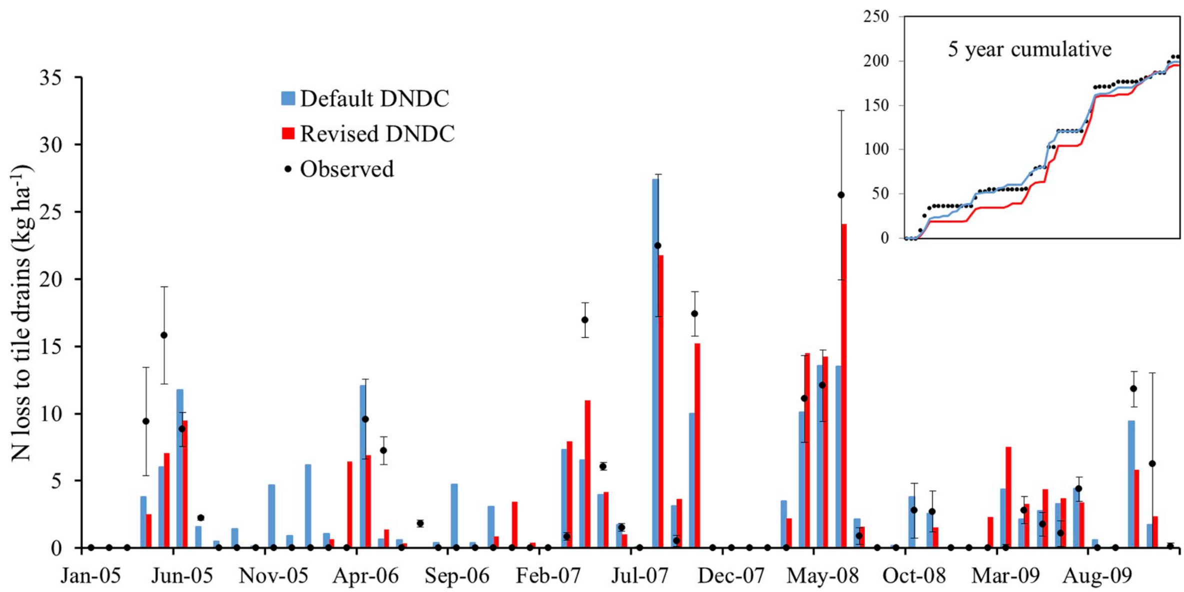

Fig. 5. Comparison of monthly simulated N loading to tiles using default and revised DNDC for the TD-NCC-MS validation treatment at Gilmore City.

showed "good" performance across all treatments, which was certainly satisfactory but could perhaps have been improved if additional measured soil hydraulic properties were available below 20 cm depth at the site. RZWQM2 uses the Brookes-Corey four parameter nonlinear curve fitting model for fitting water retention data and a better fit can be provided if measured saturated and residual soil water contents, pore size distribution and bubbling pressure are available. Even though revised DNDC and RZWQM2 demonstrated "good" performance in simulating drainage events, according to the d statistic, the overall magnitude of drainage was well simulated for only 3 of the treatments. For the CDS-NCC-MS treatment, observed water losses from runoff + tile drainage were considerably lower (Table S4) than for the other three treatments. Evapotranspiration was not measured but it's unlikely that there was more water loss due to ET since observed yields were similar between treatments. It is possible that there was more deep seepage, but we did not have available soil physical and hydraulic properties at deeper depths and deep seepage was assumed to be minimal (which resulted in good results for 3 of 4 treatments).

The magnitude of runoff was very well predicted over the 5 year study for all but the CDS-NCC-MS treatment, however, the statistics for simulating runoff events were "poor". Unlike default DNDC or RZWQM, the NSE was ≥ 0 for revised DNDC for all validation treatments, however, the d statistic was low. Interestingly the statistics for cumulative runoff, often being the only statistics provided by some studies (Guest et al., 2018), were "good" to "excellent", with $d \geq 0.82$ for both revised DNDC and RZWQM2 across all treatments. RZWQM2 overestimated runoff in the CDS-CC-MS treatment (Fig. 6), however as mentioned previously, the hydraulic parameters employed in the Brookes-Corey soil-water retention model are very sensitive. Below 20 cm depth these parameters were estimated using an internal curve fitting routine rather than being supplied from measured data. Note that total runoff + tile drainage were simulated with "good" model performance by RZWQM2 and "excellent" performance by revised DNDC across all treatments.

Similar to the Gilmore City location, the simulation of nitrogen loss to tiles by revised DNDC was improved over default DNDC at Woodslee and revised DNDC produced similar average statistics relative to RZWQM2 across the two CDS treatments with "fair" model performance (Table 6). Both models over-predicted N loss during the early stages of the study, then predicted less loss during 2002, with similar losses for the remainder of the study (Fig. 6). N movement to tiles in DNDC was strongly correlated with water movement (Fig. 6a and b) and overall the cumulative losses were well simulated ($d \geq 0.76$). The timing of N loss to runoff was not well simulated by either model but the cumulative loss

Table 6
Statistical performance of models for simulating water and N loss to runoff and tile drains at the Woodslee research site (n = 28 over 5 years).

Water/N component	Statistic	Calibration			Validation								
		TD-CC-MS[a]			TD-NCC-MS			CDS-CC-MS			CDS-NCC-MS		
		Default DNDC	Revised DNDC	RZWQM2	Default DNDC	Revised DNDC	RZWQM2	Default DNDC	Revised DNDC	RZWQM2	Default DNDC	Revised DNDC	RZWQM2
Tile drainage	NARE	−5.8	−0.5	−5.3	7.0	11.7	1.3	NA	5.3	−7.9	NA	59.1	25.6
	NSE	0.08	0.88	0.59	−0.06	0.85	0.59	NA	0.75	0.64	NA	0.05	0.35
	d	0.67	0.96	0.88	0.68	0.96	0.89	NA	0.94	0.89	NA	0.83	0.82
Runoff	NARE	1.5	11.3	18.9	−10.2	−5.1	0.1	NA	−0.06	57.1	NA	−26.4	12.2
	NSE	−1.85	−0.18	−0.58	−0.58	0.13	−0.26	NA	0.11	−1.62	NA	0.16	−0.37
	d	0.65	0.66	0.62	−0.71	0.64	0.55	NA	0.68	0.60	NA	0.60	0.63
Runoff + tile drainage	NARE	−4.1	1.3	0.4	2.1	6.9	1.0	NA	3.6	10.3	NA	22.7	19.9
	NSE	0.53	0.90	0.48	0.48	0.89	0.40	NA	0.90	0.39	NA	0.77	0.14
	d	0.84	0.97	0.86	0.84	0.97	0.85	NA	0.97	0.86	NA	0.95	0.82
N loss to tiles	NARE	0.9	1.2	−4.4	−1.0	14.0	4.4	NA	−1.7	18.9	NA	11.0	33.0
	NSE	0.51	0.57	0.21	0.52	0.60	0.01	NA	0.46	0.56	NA	0.20	−0.30
	d	0.79	0.82	0.70	0.81	0.88	0.77	NA	0.78	0.84	NA	0.76	0.68
N to runoff	NARE	−97.7	−5.4	−29.0	−98.0	−23.6	−42.9	NA	−13.8	−27.8	NA	−2.6	−19.6
	NSE	−0.53	−3.57	0.02	−0.77	−3.83	−0.23	NA	−3.2	−0.48	NA	−5.15	−1.20
	d	0.39	0.51	0.57	0.41	0.45	0.52	NA	0.51	0.50	NA	0.47	0.34
N to runoff + tile drains	NARE	−12.4	0.3	−7.8	−15.0	8.6	−2.5	NA	−4.8	6.8	NA	8.2	22.0
	NSE	0.49	0.55	0.21	0.50	0.66	0.06	NA	0.29	0.54	NA	0.24	−0.20
	d	0.77	0.81	0.70	0.79	0.89	0.76	NA	0.70	0.82	NA	0.76	0.69

[a] TD – unrestricted tile drainage; CDS – controlled drainage and subsurface irrigation; CC – cover crop; NCC – No cover crop; MS - Maize-soybean rotation phase; SM – Soybean-maize rotation phase.

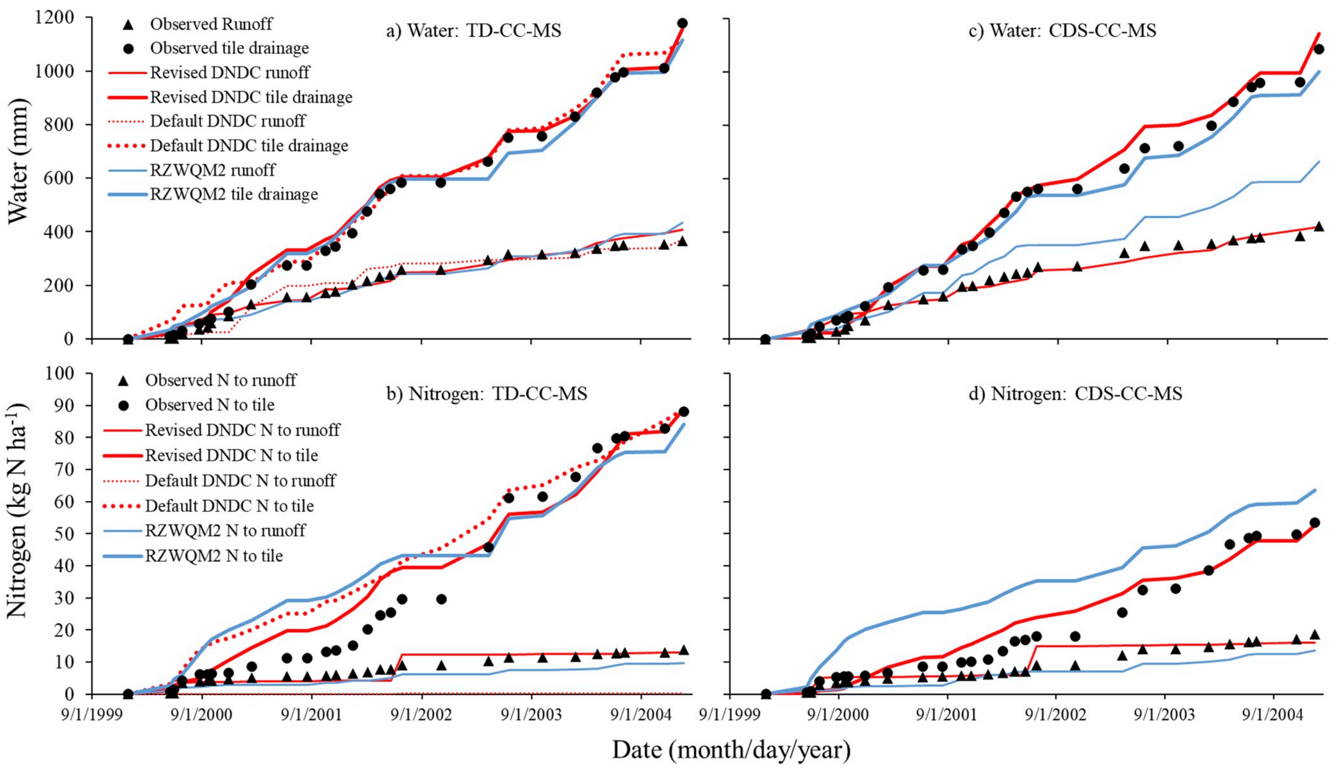

Fig. 6. Observed and simulated cumulative water and N losses to runoff and tile drains at the Woodslee research site for a) water losses using unrestricted tile drainage, b) nitrogen losses using unrestricted tile drainage, c) water losses using controlled drainage with sub-irrigation and d) nitrogen losses using controlled drainage with sub-irrigation.

was simulated with "fair" to "excellent" performance. Revised DNDC predicted a large N runoff event on June 21, 2002 at the time of 66.4 mm of precipitation which was not observed nor predicted by RZWQM2. It is likely that DNDC under-predicted the rate of N movement down the profile with too much N remaining in the top 2 layers (~3 cm depth). Note that default DNDC predicted nearly zero N in runoff as the fraction of N lost to runoff was set internally at a very low value and was only based on the top soil layer.

Revised DNDC simulated the appropriate reduction in N losses to tiles under controlled drainage relative to unrestricted drainage (Fig. 6, Table S4). The reduction in N loss to drains from CDS for the CC treatments was −39.1%, −40.8% and −24.3% for observed, revised DNDC and RZWQM2, respectively (Fig. 6, Table S4), whereas CDS reduced nitrate loss by −37.5%, −39.1%, and −20.2% for the NCC treatments compared to unrestricted tile drainage (Table S4). Reduced N loss to tiles for controlled drainage relative to unrestricted drainage is a common finding in many studies (Drury et al., 2009, 2014; Tan et al., 1993, 2007). Since soil N is a crucial driver for several biogeochemical processes, the successful simulation by revised DNDC expands the models accuracy and capabilities.

4. Conclusions

Inaccuracies in the simulation of water and N dynamics in the DNDC model have strongly impacted and impeded the further development of several related biogeochemical processes, particularly in the case of trace gas emission estimates. Prior to the developments implemented in this study, DNDC (Canada & U.S. versions) only simulated cascade water flux vertically down the soil profile without a mechanistic tile drainage algorithm. We implemented a deeper and heterogeneous soil profile, root penetration and density functions, a fluctuating water table, unsaturated flow above field capacity, and the Hooghoudt equation to simulate mechanistic tile drainage based on drain spacing, depth and tile diameter. After development, simulations of soil water storage, daily drainage, N loss to runoff and N loss to tile drains were improved, comparing well to measurements at two research sites and showing at least as good of performance as RZWQM2. This demonstrated that DNDC development was successful considering RZWQM2 is a well-validated water quality model which includes detailed computational hydrology. The soil-water input requirements for DNDC were kept relatively low and the model simulation time remains 4 times faster than RZWQM2, which are important factors for larger scale assessments. The revised DNDC model did not simulate the timing of water or N losses to runoff well but performed satisfactory in simulating the cumulative magnitudes. The simulation of runoff is complex particularly when surface crusting, clay cracking, preferential flow through insect and root channels, snow dynamics, and soil freeze-thaw are prevalent and further research is recommended. Through these developments we have expanded the ability of DNDC to simulate the impacts of tile drainage management such as drain depth and spacing, controlled drainage and sub-irrigation on soil water and N dynamics. Future studies should now focus on improving biogeochemical processes such as nitrification, denitrification, fermentation and mineralization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envsoft.2019.104577.

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