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Winter rye as a cover crop reduces nitrate loss to subsurface drainage as simulated by HERMES

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ABSTRACT

HERMES is a widely used agricultural system model; however, it has never been tested for simulating N loss to subsurface drainage. Here, we integrated a simple drain flow component into HERMES. We then compared the predictions to four years of data (2002–2005) from central Iowa fields in corn-oybean with winter rye as a cover crop (CC) and without winter rye (NCC). We also compared the HERMES predictions to the more complex Root Zone Water Quality Model (RZWQM) predictions for the same dataset. The average annual observed and simulated N loss to drain flow were 43.8 and 44.4 kg N/ha (NCC) and 17.6 and 18.9 kg N/ha (CC). The slightly over predicted N loss for CC was because of over predicted nitrate concentration, which may be partly caused by slightly under predicted average annual rye shoot N (observed and simulated values were 47.8 and 46.0 kg N/ha). Also, recent research from the site suggests that the soil field capacity may be greater in CC while we used the same soil parameters for both treatments. A local sensitivity analysis suggests that increased field capacity affects HERMES simulations, which includes reduced drain flow nitrate concentrations, increased denitrification, and reduced drain flow volume. HERMES-simulated cumulative monthly drain flow and annual drain flow were reasonable compared to field data and HERMES performance was comparable to other published drainage model tests. Unlike the RZWQM simulations, however, the modified HERMES did not accurately simulate the year to year variability in nitrate concentration difference between NCC and CC, possibly due in part to the lack of partial mixing and displacement of the soil solution. The results suggest that 1) the relatively simple model HERMES is a promising tool to estimate annual N loss to drain flow under corn-soybean rotations with winter rye as a cover crop and 2) soil field capacity is a critical parameter to investigate to more thoroughly understand and appropriately model denitrification and N losses to subsurface drainage.

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1. Introduction

The agricultural system model HERMES has been part of several international model intercomparisons and recent large model ensembles testing simulated wheat and maize growth (De Willigen, 1991; Diekkrüger et al., 1995; Kersebaum et al., 2007; Bassu et al., 2014; Palosuo et al., 2011; Kollas et al., 2015; Martre et al., 2015; Asseng et al., 2013, 2015; Eitzinger et al., 2013). In comparisons of multiple crop growth models such as DSSAT-CERES, DAISY, and STICS, HERMES has been reported among the top performers (Rötter et al., 2012; Palosuo et al., 2011; Asseng et al., 2015). HERMES has also been shown to accurately simulate N dynamics for a range of field conditions and crop rotations in the Czech Republic (Hlavinka et al., 2014) and used to optimize nitrogen management in Germany and the North China Plain (Kersebaum and Beblik, 2001; Kersebaum et al., 2005; Herrmann et al., 2005; Michalczyk et al., 2014). The model, however, has not been used or tested for simulating N loss to artificial subsurface drainage, and the model has not been tested for simulating N leaching in the U.S.

HERMES has participated in several model ensembles inlcuding the Agricultural Model Intercomparison and Improvement Program (AgMIP; Asseng et al., 2013, 2015). The mission of AgMIP “is to significantly improve agricultural models and scientific and technological capabilities for assessing impacts of climate variability and change and other driving forces on agriculture, food security, and poverty at local to global scales.” (AgMIP, 2016). The demand for corn and soybean is projected to increase with an increasing world population that is more prosperous and has higher per capita

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meat consumption (e.g., Godfray et al., 2010). With increased food demand, increased use of N-fertilizer will be required under nearly all possible scenarios (Cassman et al., 2003). On the other hand, anthropogenic perturbation of the global nitrogen (N) cycle is of increasing concern, and contributes to hypoxia, loss of biodiversity, and habitat degradation in coastal ecosystems (Galloway et al., 2003; Gruber and Galloway 2008; Canfield et al., 2010). Cover crops grown after the main crop harvest are a promising method to substantially reduce nitrate contamination from leaching below the soil root zone and from leaching to subsurface drains (Kaspar et al., 2007, 2008, 2012; Martinez and Guiraud, 1990; Shepard, 1999). Reducing excess nitrate loss to artificial "tile" drains in the U.S. Midwest is important for reducing excessive nitrate in the Mississippi River, which has been identified as a leading cause of hypoxia in the northern Gulf of Mexico (Rabalais et al., 1996; EPA-SAB, 2007). And the area within the Mississippi River watershed, identified by Goolsby et al. (2001) as the primary source of nitrate to the Gulf, is the same area where corn production on artificially drained lands is prevalent. A fall-planted "winter" cover crop may help reduce the hypoxic zone in the Gulf of Mexico and elsewhere if implemented on a large scale (Malone et al., 2014a; Kladivko et al., 2014).

Agricultural models can be useful to simulate and help evaluate the effects of management practices, including winter cover crops, under a wide range of pedoclimatic conditions but they must be tested for the accuracy of their predictions compared to measured data (Constantin et al., 2015, 2012; Kersebaum et al., 2015). Furthermore, testing models against field data where cover crops are included in the rotation is important because the capability of crop models to simulate cover crops is somewhat limited due to a lack of information concerning model parameterization and use (Kollas et al., 2015). Li et al. (2008) tested the Root Zone Water Quality Model (RZWQM) using field data from a central Iowa site and concluded that RZWQM was a promising tool to estimate the relative effects of winter rye as a cover crop on nitrate loss reduction to drain flow. Following the promising results of Li et al. (2008), RZWQM has been used to simulate the effects of winter rye in reducing N loss to drainage at several Iowa locations as well as across the U.S. Midwest (Qi et al., 2011; Singer et al., 2011; Malone et al., 2014a). Agricultural system models other than RZWQM such as STICS, DSSAT, and SWAT have been recently tested and/or used to simulate the effect of cover crops in reducing N leaching (Constantin et al., 2015; Salmeron et al., 2014; Yeo et al., 2014). The HERMES model has been used to simulate growth of cover crops other than rye or growth of rye as a main crop (Kersebaum, 2007). However, HERMES has not been tested against field data for the effects of winter rye as a cover crop on reducing N loss to subsurface drainage.

Studies comparing different models for simulating nitrate losses to subsurface drainage can be useful to identify model strengths and weaknesses as well as to identify appropriate model complexity for specific purposes. Model comparisons have been conducted for predicting targets such as crop growth, nitrogen dynamics, and pesticide loss (e.g., De Willigen, 1991; Jamieson et al., 1998; Kersebaum et al., 2007; Palosuo et al., 2011; Armstrong et al., 2000; Ma et al., 1998). Few studies, however, have compared different agricultural system models for simulating the effects of winter cover crops on nitrate loss to artificial subsurface drainage. Ale et al. (2013) compared the performance of DRAINMOD to previous simulations of ADAPT by Davis et al. (2000) for nitrate loss to subsurface drainage under continuous corn in southern Minnesota. Thorp et al. (2009) compared the performance of DRAINMOD to previous simulations of RZWQM by Thorp et al. (2007) for nitrate loss to subsurface drainage under corn-soybean systems with different nitrogen fertilizer rates. Although HERMES has been used to simulate N dynamics in places such as Germany, the Czech Republic, and China (Kersebaum, 2007; Hlavinka et al., 2014; Michalczyk et al., 2014) and compared to other models for crop growth and nitrogen leaching (Rötter et al., 2012; Kersebaum et al., 2007), it has not been compared to other models for simulating nitrate leaching to subsurface drains. RZWQM has been used to estimate the effects of winter rye as a cover crop to reduce N loss to drain flow across the U.S. Midwest and has been shown to be a promising tool to estimate the effects of winter rye (Malone et al., 2014a; Li et al., 2008). However, the effect of winter rye on reducing N loss to drainage was under predicted in these studies. Comparing the simulation results of Li et al. (2008) to HERMES could help determine if the RZWQM under predicted winter rye effect was RZWQM specific or if it is more systematic of agricultural system models.

Less complex models such as HERMES with fewer adjustable parameters may have some advantages compared to more complex models such as RZWQM. As early as 1975 hydrologic model comparison has been an important research topic (WMO, 1975). Scientific contributions following this World Meteorological Organization (WMO) model comparison include Naef (1981) concluding that simple models may provide simulations of runoff in small basins as satisfactorily as more complex models. More recently, scientific objectives of large international projects such as AgMIP include intercompare crop and agricultural models with observed field trials in order to identify model strengths, weaknesses, and uncertainties (Rosenzweig et al., 2013). Diekkrüger et al. (1995) reported that simple agroecosystem models may lead to better results than those computed from a complex model. Perrin et al. (2001) reported that the hydrologic models in their study with fewer adjustable parameters performed as well as more complex models on the verification datasets, and that increased model complexity could result in hydrologic model over parameterization and increased parameter uncertainty. Similarly, Michaud and Sorooshian (1994) reported that when calibration was performed, the accuracy of a complex distributed runoff model was similar to that of a simple distributed model. Part of the complexity of RZWQM is that it simulates soil water redistribution using soil water potential, which requires more than ten adjustable parameters to describe the soil physical characteristics of each soil layer (e.g., saturated hydraulic conductivity, porosity, Brooks-Corey water retention and unsaturated hydraulic conductivity parameters). HERMES, on the other hand, uses a capacity water flow model that requires three adjustable soil physical characteristic parameters (field capacity, wilting point, porosity). In developing the simple pesticide fate model LEACHA as an alternative to the complex model LEACHP, Hutson and Wagenet (1993) discussed that "most model complexity in soil-water-chemical simulation models arises from the manner in which water flow and chemical transport are considered". Hutson and Wagenet (1993) go on to state "with the advent of large-scale assessments using GIS and soil survey data bases to estimate leaching, it is important to accelerate the development of simplified, yet acceptably accurate pesticide leaching models that minimize input data requirements". Buttler and Riha (1992) reported that both capacity and potential-driven water movement models produced similar estimates of seasonal drainage, evaporation, and transpiration. In addition to the complexity and large number of input parameters to determine and input, another disadvantage of potential-driven water movement models is that the solution of the partial differential equation is highly nonlinear and the numeric solution can fail to converge (Short et al., 1995). Lack of numeric convergence for certain combinations of variable inputs is problematic with the increased use of automatic model calibration packages such as PEST where many thousands of computer runs may be necessary for automatic model calibration (Doherty, 2004). Therefore, use of a less complex model such as HERMES could: 1) have similar or improved results to more complex models (Diekkrüger et al., 1995; Michaud and Sorooshian, 1994); 2) reduce the potential for model "over parameterization" (Perrin et al., 2001); 3) have less parameters to input and be more applicable for areas where knowledge on soil properties is limited (Hutson and Wagenet, 1993) and; 4) have less problems associated with numeric convergence. Despite the conditional advantages of capacity-driven water movement models, more complex soil water potential-driven models are more mechanistic with advantages that include (Seyfried, 2003): 1) allowing for the study of processes involved in soil water movement; 2) in principle, can be transferred to any site because the processes are universal; and 3) in principle, can be used to more mechanistically simulate related processes such as plant water uptake and solute transport.

In summary, although HERMES is a widely used agricultural system model, it needs to be tested for simulating N loss to subsurface drain flow under multiple practices including winter cover crops and it needs to be compared to more mechanistic soil water/solute models for simulation of N loss to subsurface drainage. Here, we integrated a simple drain flow component into HERMES and applied it to a corn-soybean rotation in central Iowa. The research objectives were to compare the HERMES simulated and field observed effects of a winter rye cover crop on nitrate losses in an artificially drained corn-soybean rotation using the same dataset as Li et al. (2008). We also compare the results of the relatively simple HERMES model to the more complex RZWQM as reported by Li et al. (2008) using the same data. As part of this study we evaluated the simulated nitrogen budget and conducted a local sensitivity analysis.

2. Materials and methods

2.1. Field used to test model and management

The Boone County Iowa field experiment used to test HERMES for response to winter rye was described in detail by Malone et al. (2014a), Li et al. (2008), and Kaspar et al. (2007), which included description of soils plot design, management, and field measurements. The field management as input into HERMES is summarized in Table 1. The actual rye planting dates in fall of 2001 and 2002 were earlier than input into HERMES because the model does not currently simulate intercropping. Also, an earlier rye termination date was entered into HERMES than occurred in the field for spring 2003 to address the poor rye establishment, which HERMES does not simulate. The 2003 rye termination date was set to simulate N uptake by winter rye in spring 2003 similar to Li et al. (2008) and average annual 2002–2005 N uptake similar to field observations.

2.2. Model description and comparison

Detailed descriptions of RZWQM and HERMES model components have been reported elsewhere (Ma et al., 2001; Kersebaum and Beblik, 2001; Ma et al., 2011; Kersebaum, 2011; Kersebaum et al., 2005; Ahuja et al., 2000). We briefly describe the water, C/N cycling/movement, and crop components of the two models, which are summarized in Table 2.

For RZWQM, rainfall or snowmelt is received by the soil surface. Snow dynamics are simulated by an adaption of the PRMS model (Leavesley et al., 1983) that includes accumulation and depletion using an energy and water budget approach (Ahuja et al., 2000). Water infiltrates into the soil according to the Green-Ampt equation and water redistribution occurs according to potential and a numerical solution to the Richards' equation. Subsurface drainage is simulated according to the Hooghoudt's equation while rainfall and snowmelt in excess of infiltration and macropore flow is directed to runoff. Potential ET is simulated with a modification of the Shuttleworth-Wallace that includes the effects of surface residue. HERMES does not simulate runoff or snowmelt. To partially compensate, rainfall was entered into HERMES from the RZWQM simulated daily rainfall and snowmelt. HERMES simulates soil water movement using a modified capacity (tipping bucket) approach that includes capillary rise from shallow groundwater and subsurface drainage as a user defined fraction of percolate at the drain line depth. HERMES does not simulate ET as a function of surface residue, but it does offer several potential ET options and includes a module to simulate soil temperature (Kersebaum, 2011).

The HERMES model was modified to include a simple drainage component that uses a user defined drainage fraction (Table 2) to divide percolating water between deep percolation below the user defined drainage layer and subsurface "tile" drainage. Drain flow occurs when field capacity is exceeded in the drainage layer and N loss in the drainage is derived from the N concentration of soil water in the drainage layer.

The C:N module in RZWQM simulates two plant residue pools, three soil humus pools, and three soil microbial pools. The different residue and humus pools decay at different rates (slow to fast). Each residue or humus pool is subject to first order decay as a function of carbon content, the heterotrophic microbial population, and soil environmental variables such as soil water content and temperature. Nitrogen is released during the decay process as NH_4 and may be nitrified to NO_3 following a zero order equation as a function of soil environmental variables and the autotrophic microbial population. Nitrate from nitrification or applied fertilizer is subject to denitrification under anaerobic conditions according to a first order equation as a function of soil environmental variables and the anaerobic microbe population. The microbial biomass is subject to death and growth. HERMES simulates net N mineralization from two pools of decomposable soil organic matter (fast and slow decay) according to a first order equation as a function of soil temperature and water content. Denitrification is simulated with HERMES from the top 30 cm of soil using Michaelis-Menten kinetics modified for soil temperature and soil water content. Solute transport with RZWQM is achieved with a partial mixing and displacement approach while HERMES uses convection-dispersion.

The results and discussion below identify denitrification as an important process associated with HERMES simulated N loss to subsurface drainage that is sensitive to soil field capacity and porosity. HERMES simulated denitrification was presented previously (Kersebaum, 1995) and we briefly describe it here. The denitrification loss rate (DN/t, kg N/ha/day) is calculated as a function of the soil nitrate content (NO3, kg N/ha), relative soil water saturation (RSWS = soil water content divided by soil porosity), and the soil temperature (T) of the upper 30 cm by

$$DN/t = Vmax \times (NO3)^2 \times [(NO3)^2 + KN]^{-1} \times \{1 - \exp[-(RSWS/CSWS)^6]\} \times \{1 - \exp[-(T/CT)^{4.6}]\} \quad (1)$$

Where V_{max} is the maximum denitrification loss per unit time (1.274 kg N/ha/day), CSWS and CT are critical values for soil water saturation and temperature below which a strong reduction of denitrification occurs (77% and 15.5 °C), and KN is a Michaelis-Menten type coefficient (74 $[\text{kg N ha}^{-1}]^2$)

Numerous plant growth options are available in RZWQM (Ma et al., 2011; Table 2). The CROPGRO option was used for soybean and CERES was used for corn and winter rye (Li et al., 2008; Thorp et al., 2007). HERMES simulates crop growth using a generic approach that can simulate different crops using external crop parameter files and is based on the SUCROS model (Van Ittersum et al., 2003; Van Keulen, 1982). Legume crops such as alfalfa have been simulated previously by HERMES that included estimating nitrogen fixation as the crop N demand in excess of soil availability (Hlavinka et al., 2014). Modifications for soybean included adjusting the daylength parameter for each growth stage to account for the short-day requirements of soybean, which resulted in initiating flowering during early July most years. Compared to the

Table 1
Field operations entered in HERMES.

Crop	Sowing date	Main crop harvest and rye termination	Fertilizer application date	N amount (kg N/ha)
Corn	May 1, 2000	Oct 1, 2000	Apr 14, 2000	224
rye	Oct 5, 2000	Apr 16, 2001		
Soybean	May 10, 2001	Sept 28, 2001	June 20, 2001	1
Rye	Sept 30, 2001	Apr 17, 2002		
Corn	Apr 25, 2002	Sept 30, 2002	May 2, 2002	13
				224
Rye	Oct 2, 2002	Apr 20, 2003	May 30, 2002	
Soybean	May 12, 2003	Sept 30, 2003	June 17, 2003	1
Rye	Oct 2, 2003	Apr 16, 2004	Oct 3, 2003	16
Corn	Apr 28, 2004	Oct 4, 2004	Apr 28, 2004	13
Rye	Oct 6, 2004	Apr 25, 2005	May 21, 2004	217
Soybean	May 5, 2005	Sept 30, 2005	Nov 23, 2005	40
Rye	Oct 3, 2005	Apr 21, 2006		

Table 2
Comparison of processes simulated in RZWQM2 and HERMES models.

Processes/system components	RZWQM2	HERMES
Snow dynamics	PRMS approach	Not considered
Water infiltration	Green-Ampt equation	Unlimited
Runoff	Amount that exceeds soil matrix infiltration and macropore flow	Not considered
Subsurface drainage	Hooghoudt's steady state equation	Defined fraction
Water redistribution	Soil water potential with Richards' Equation	Modified capacity approach "tipping bucket"
Potential ET	Modified Shuttleworth-Wallace that includes surface residue effects.	Penman-Monteith, optional Priestley-Taylor, Turc-Wendling or externally calculated
N movement in soil	Partial displacement	Convection-dispersion
Soil C/N processes	Mineralization, immobilization, nitrification, denitrification, urea hydrolysis, methane production, N2O emission, ammonia volatilization, microbial growth and death. 2 residue pools, 3 humus pools, and 3 microbial pools.	Net mineralization, denitrification, urea hydrolysis, ammonia volatilization. 2 decomposable N pools.
Plant Growth	Several options are available that include: CROPGRO; CERES; QUICK PLANT for simple and limited parameter input plant, turf, and tree growth	Based on SUCROS

CROPGRO/CERES models, which use a simple radiation use efficiency (RUE) approach, HERMES simulates daily crop growth based on the photosynthesis minus respiration approach (Asseng et al., 2013). Yield is estimated from the partitioning during the relevant growth stages without a defined harvest index. While root water uptake in the CERES approach uses water potential inside and outside roots, HERMES uses an approach relating water uptake to plant available water and root length density (Wu and Kersebaum, 2008). Nitrogen uptake with CERES uses plant available water, a maximum uptake per root length and available nitrogen, while HERMES uses a radial convection diffusion approach to consider limitation of N supply during drought periods.

2.3. Model calibration and testing

For HERMES calibration and testing, two individual plots were used. One was a control treatment plot without winter rye included as a cover crop (NCC). The other had the same field operations as the control plot (NCC) except that a winter rye cover crop was included (CC). In addition to the rye and no rye of these two plots, these plots were chosen partly because they had annual drain flow and nitrate concentrations in drain flow near the middle of the four replicates. It was decided to calibrate and test the model using only two plots rather than the average of the four replicates because the timing of drain flow starting, stopping, and collection of samples were not synchronized among replicates. We do compare the HERMES simulated annual drainage, flow weighted nitrate concentration in drainage (FWNC), and N loss to drainage to the standard deviation of the four replicate plots.

HERMES was calibrated for NCC and tested using CC. Model input includes meteorological data (rainfall, temperature, wind speed, solar radiation, and humidity) collected from a weather station located 5.4 km southwest of the study area. The model simulation was started in 1992 to allow hydrology and C/N dynamics to initialize prior to model calibration and was tested using data from 2002 to 2005. For the initialization period, soybean was planted in odd years and corn in even years with fertilizer input in even years as 160 kg N/ha on April 30 from 1992 through 1998.

Model calibration included adjusting selected parameters to optimize NCC for annual and monthly subsurface drain flow, composite nitrate concentration in drain flow, and nitrate loss to drain flow. Other model output in the optimization included corn and soybean harvest yield and corn and soybean biomass. Rather than reserve part of the NCC data for model testing, we calibrated hydrology and plant growth using all four years of observed data similar to the RZWQM calibration from Li et al. (2008). Youssef et al. (2006) also calibrated DRAINMOD-N II using a 6-year dataset from one plot and tested the calibrated model using different plots. Although HERMES allows soil parameter values at 10 cm resolution, we input one value for the 2 m soil profile for each of the soil properties field capacity, wilting point, and porosity. The field values would normally vary with depth, but using a single "effective "value for the profile resulted in acceptable simulations compared to observed data. Interpreting all the layers in the soil profile as a single unit may be similar to the common practice of interpreting the field as a single unit (e.g., single soil type) with effective parameters to simplify heterogeneity (Djurhuus et al., 1999; Hansen et al., 2012; Skaggs et al., 2012; Malone et al., 2015).

These optimized parameters were used in CC without adjusting. The final optimized parameters are listed in Table 3 and were constrained to a range of values that were reasonable for the conditions. Winter rye parameters for HERMES were taken from Graß et al. (2015). The initial crop coefficient (Kc) for simulation of actual evapotranspiration under winter rye was adjusted for site specific conditions. The only other winter rye parameter adjusted was the increased root growth speed. This resulted in HERMES slightly over predicting simulated rye shoot dry mass and slightly under predicting shoot N as discussed below. With only four years of field

Table 3
Calibrated HERMES input parameters.

Parameter	Value	Comments and Justification.
Field capacity (cm^3/cm^3)	0.284	Rawls et al. (1982) lists the range for clay loam of 0.25–0.39.
Wilting point (cm^3/cm^3)	0.145	Rawls et al. (1982) lists the range for clay loam of 0.11–0.28.
Porosity (cm^3/cm^3)	0.453	Rawls et al. (1982) lists the range for clay loam of 0.41–0.52. Li et al. (2008) input porosity of 0.49 at 10 cm–0.36 at 200 cm. Therefore our values are reasonable with using one effective value for the entire soil profile.
Fraction of organic matter that is available for slow decay	0.12	Default is 0.13 (e.g., Kersebaum, 1995)
AMAXS (kg CO_2/ha leave/h) AMAXC (kg CO_2/ha leave/h) AMAXR (kg CO_2/ha leave/h)	20.083.865.0	Soybean, corn, and winter rye maximum CO_2 assimilation rates are AMAXS, AMAXC, and AMAXR. AMAXR is the same as Graß et al. (2015).

Additional calibrated input parameters include the Fraction of percolate lost to drainage (0.75) and the Fraction of applied fertilizer that is volatilized (0.05). Soil organic carbon (%) was input similar to unreported values from Li et al. (2008): 3.3, 2.5, 1.3, 0.5, and 0.0 for 10, 20, 150, 160, and 200 cm.

measured rye biomass and shoot N at spring termination, we did not thoroughly test the rye growth component of HERME Li et al. (2008) also did not thoroughly test RZWQM for rye growth.

The optimization combined both manual parameter adjustment and the first use of the automatic parameter estimation (calibration) program PEST (Doherty, 2004) linked to HERMES. One of the advantages of utilizing PEST is that all HERMES input parameters listed in Table 3 could be adjusted simultaneously to minimize a multi-criteria objective function composed of 7 different observation groups: annual and monthly drain flow volume (cm); annual and monthly flow weighted nitrate concentration in drainage (mg N/L); annual N loss to drain flow (kg N/ha); annual corn and soybean yield (kg/ha) and biomass (kg/ha). The PEST optimization linked to RZWQM was described by Malone et al. (2014b, 2010).

One of the main indicators used for model evaluation is the Nash-Sutcliffe efficiency (EF, Nash and Sutcliffe, 1970), which was used and defined by Li et al. (2008). Model simulations can be considered satisfactory under a monthly time step if EF >0.5 (Moriasi et al., 2007). The value of EF when model estimates perfectly match observed data is 1.0. Values for EF less than zero indicate that the average of observed measurements were a better estimator than the model. The Relative Root Mean Square Error (RRMSE; RMSE/$\overline{O}$) was also used as a performance indicator. Other applied indicators of model performance included plotting and/or discussing: cumulative drainage volume and N loss to drain flow (Branger et al., 2009; Youssef et al., 2006); observed and simulated average annual flow weighted nitrate concentration (FWNC) differences in drainage between NCC and CC (Li et al., 2008); annual HERMES simulated drain flow volume, N loss to drainage, and nitrate concentration predictions compared to the standard deviations of the four field replicates; and observed and simulated average annual N loss to drain flow differences between NCC and CC (Li et al., 2008). Some important components of the hydrologic and N budgets were not measured and are discussed in comparison to literature-determined or expected values for the site conditions: ET, mineralization, and denitrification. The statistical performance indicators in this paper focus on an annual time period to match Li et al. (2008).

2.4. Sensitivity analysis

A local sensitivity analysis was performed for five soil-related model input parameters and the corn growth coefficient AMAXC (Table 3) on three model outputs: annual N loss to drain flow, annual FWNC, and drain flow volume. Sensitivity of models other than HERMES that simulate winter cover crop such as the models RyeGro, APSIM, and RZWQM have been analyzed for: 1) crop or weather variables effect on rye cover crop growth (Feyereisen et al., 2006), 2) cover crop root depth and critical N concentration limits effect on N loss to drainage (Malone et al., 2007), and weather and management effect on N loss to drainage with winter rye cover crop (Malone et al., 2014a). This is the first study, however, to analyze HERMES simulated winter cover crop effect on N loss to drainage from soil- and crop-related parameter changes. The parameters evaluated were: field capacity, wilting point, porosity, fraction of organic matter that is available for slow decay, drainage fraction, and the coefficient controlling the maximum CO_2 assimilation rate for corn (AMAXC). Relative sensitivity coefficients (Sr) were determined (see Feyereisen et al., 2006):

$$Sr = (O_{P+dP} - O_{P-dP}) * O^{-1} * (2 * dP/P)^{-1},$$

where O is the model output with input parameters at base values; O_{P+dP} and O_{P-dP} are the model outputs with the input parameter adjusted from the base value by a specified percentage (about 10% in our case); P is the initial value of the input parameter, and dP is the change in the value of the input parameter.

The purpose of the sensitivity analysis was to identify the soil-related parameters that have the greatest influence on model results and to determine the effect of corn growth on selected model output. To gain further insight into the effect of parameters on model results, the parameter with the greatest sensitivity was evaluated for the annual N budget changes compared to using the base parameter values (N uptake by crops, mineralization, denitrification, N loss to drainage, fixation, and annual soil N change).

3. Results and discussion

3.1. Model performance

Overall HERMES reasonably simulated annual N loss in NCC and CC compared to field observed data and reasonably simulated the annual differences between the two treatments (Fig. 1). The average annual observed and simulated N losses were 43.8 and 44.4 kg N/ha for NCC and 17.6 and 18.9 kg N/ha for CC (Table 4), with an overall EF including both treatments of 0.76 (n = 8; Fig. 1).

The monthly N loss was simulated reasonably well compared to observed data (Figs. 2 and 3; EF >0.48 and R^2 >0.47 for each treatment). The simulated monthly N loss was not closer to field observations partly because predicted drain flow was occasionally incorrect during the fall months as discussed in Section 3.1.4. The cumulative monthly N loss over the four year period was simulated well compared to observed data (fig. 2; EF >0.95 for each treatment), with NCC over predicted by 2% (2.8 kg N/ha) and CC over predicted by 8% (5.3 kg N/ha). In comparison, Youssef et al. (2006) reported excellent DRAINMOD-N simulations with cumulative predicted NO_3–N leaching losses over a six year period within 8.1% of observed (18.3 kg N/ha).

HERMES slightly under predicted the average annual effect of winter rye reducing N loss to drainage with observed and simulated

Table 4
Annual observed (Obs) and HERMES (HE) simulated results for the Boone County, Iowa, field experiment with winter rye used as the cover crop treatment. A summary of the Li et al. (2008) results are also presented for the RZWQM (RZ) simulations at the same site and time period.

Year	Crop Constituents											
	Main crop yield (Mg/ha)				Cover crop shoot dry mass (Mg/ha)				Cover crop shoot N (kg N/ha)			
	NCC		CC		NCC		CC		NCC		CC	
	obs	HE	obs	HE	obs	HE	obs	HE	obs	HE	Obs	HE
2002	10.5	10.5	9.5	10.5	–	–	2.4	2.6	–	–	56	57.1
2003	2.4	3.6	2.4	3.6	–	–	0.3	1.3	–	–	9	43.0
2004	11.2	12.1	11.3	12.1	–	–	1.5	2.0	–	–	49	47.1
2005	3.9	3.8	3.6	3.8	–	–	2.7	2.5	–	–	77	36.7
Ave.	7.0	7.5	6.7	7.5	–	–	1.7	2.1	–	–	47.8	46.0

Year	Water constituents											
	Drain flow amount (cm)				Flow weighted nitrate concentration (FWNC; mg N/L)				Nitrate loss to drain flow (kg N/ha)			
	NCC		CC		NCC		CC		NCC		CC	
	obs	HE	obs	HE	obs	HE	obs	HE	obs	HE	Obs	HE
2002	18.0	12.3	18.7	8.6	17.0	14.0	4.3	9.0	30.6	17.1	8.0	7.8
	(14.7)[a]		(5.1)		(3.3)		(3.3)		(19.7)		(3.9)	
2003	31.4	31.1	29.4	27.6	22.5	26.2	10.8	10.8	70.7	81.6	31.8	29.7
	(12.6)		(4.7)		(5.9)		(5.4)		(14.0)		(9.7)	
2004	25.5	29.6	27.1	26.6	18.0	20.7	8.3	11.6	45.9	61.2	22.4	30.8
	(10.1)		(6.1)		(3.0)		(2.3)		(12.4)		(4.2)	
2005	15.0	16.2	15.4	11.4	18.5	10.9	5.3	6.5	27.8	17.6	8.1	7.4
	(11.9)		(6.8)		(4.8)		(3.5)		(18.0)		(7.7)	
AveEFR2RRMSE	22.5	22.3	22.6	18.6	19.0	17.9	7.2	9.5	43.8	44.4	17.6	18.9
	0.69		0.11		−3.96		−0.30		0.45		0.82	
	0.83		0.89		0.56		0.49		0.92		0.87	
	16.0		24.2		24.8		40.9		28.9		24.5	

Year	Summary of Li et al. (2008) water constituent simulations											
	Drain flow amount				FWNC				Nitrate loss to drain flow			
	NCC		CC		NCC		CC		NCC		CC	
	obs	RZ	Obs	RZ	obs	RZ	obs	RZ	obs	RZ	Obs	RZ
Ave	24.9[b]	23.8	22.6	18.5	21.3	18.2	8.7	9.3	50.8	44.8	19.8	19.3
EF	0.53	–	−0.01	–	−2.05	–	0.64	–	0.48	–	0.82	–
R2	–	–	–	–	0.62	–	0.86	–	–	–	–	–
RRMSE	17	–	27	–	18	–	15	–	26	–	20	–

[a] The observed standard deviation of the annual water constituent data is in parentheses.
[b] The average annual observed values reported by Li et al. (2008) are different than the current values because they used the average of the four replicates. The current analysis uses plot 16 (NCC) and 20 (CC) observed values (see section 2.3).

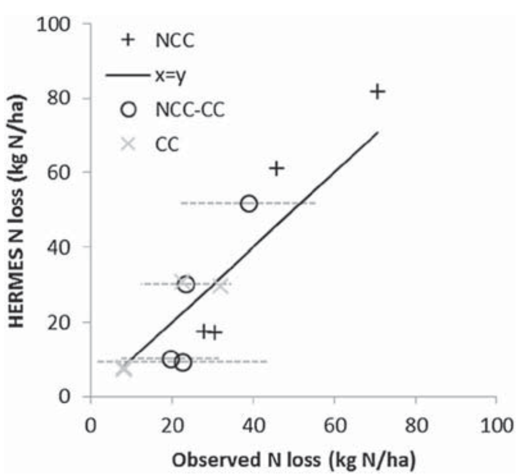

Fig. 1. Annual N loss to drain flow. CC is cover crop treatment; NCC is control treatment (no cover crop). The circles are the annual N loss difference between NCC and CC. The line is x = y; the error bars are the standard deviation of the observed data.

NCC-CC differences of 26.2 and 25.5 kg N/ha (Table 4). In our case the slight over predicted N loss for CC was mostly because of over predicted nitrate concentration and not because of over predicted drain flow (drain flow was under predicted for CC; Table 4). Some of the possible reasons for this will be discussed below.

3.1.1. *Corn and soybean*

Average annual corn yield was over predicted by 0.4 Mg/ha and the higher observed and simulated corn yield was in 2004 (Table 4; NCC). Soybean yield was under predicted by 0.1 Mg/ha in 2005 but was over predicted by 1.2 Mg/ha in 2003 (50%) suggesting that HERMES did not respond to low precipitation in August 2003. The 2003 annual precipitation was slightly greater than the long term average, but average August precipitation was 106 mm while only 25 mm of precipitation occurred in 2003 (Kaspar et al., 2007). Also, Li et al. (2008) discussed that RZWQM over predicted soybean yield in 2003 partly because the same variety was simulated each year while different varieties were planted in the experimental plots. HERMES simulated the same main crop yield for both NCC and CC (average annual yield of 7.5 Mg/ha for both NCC and CC).

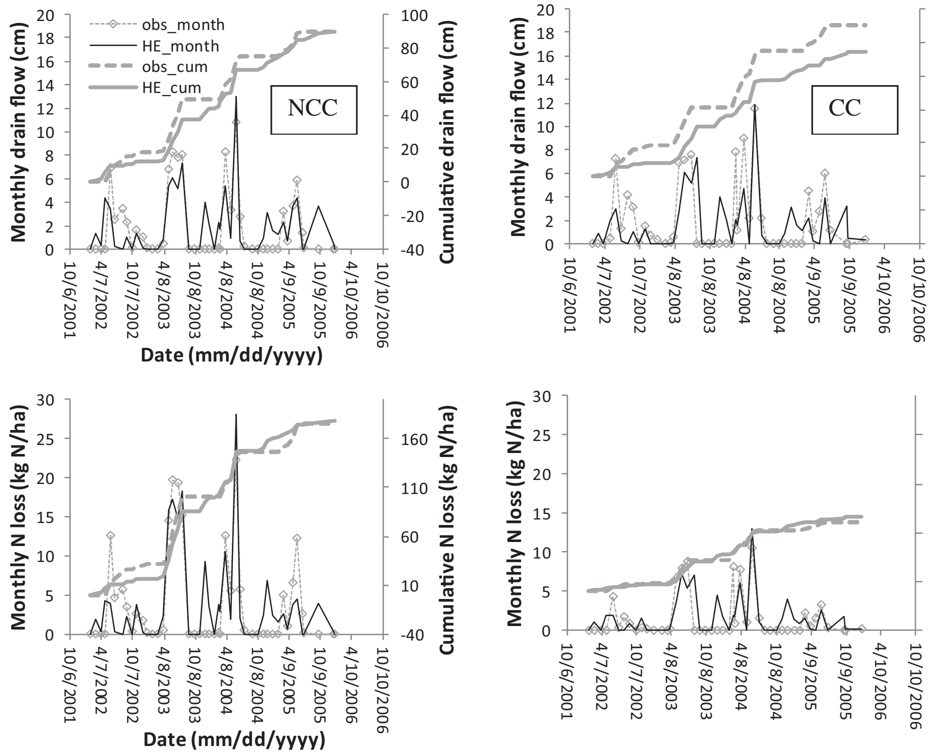

Fig. 2. Drain flow and N loss to drain flow on a monthly and cumulative monthly basis. CC is cover crop treatment; NCC is control treatment (no cover crop); obs is observed; HE is HERMES and; cum is cumulative. Note that the x-axis is scaled by sampling events and not time.

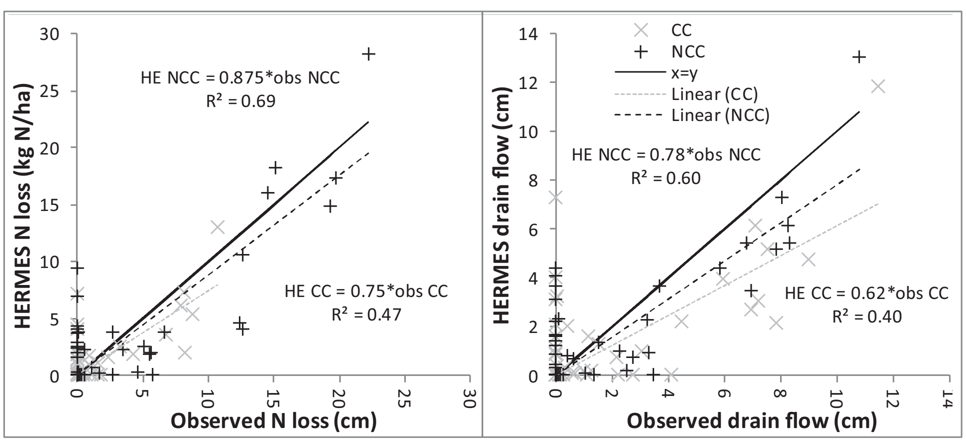

Fig. 3. Monthly drain flow and monthly N loss to drain flow. CC is cover crop treatment; NCC is control treatment (no cover crop); obs is observed and; HE is HERMES. The solid black line is x = y.

3.1.2. Winter rye

Average annual rye shoot N was under predicted by 1.8 kg N/ha or 4% compared to field data (Table 4). The least accurate shoot N estimate, excluding 2003 when planting dates were adjusted to reduce growth because of poor field establishment (see Section 2.1), was in 2005 when shoot N was under estimated by 52% (40 kg N/ha). A similar RZWQM simulated rye growth pattern was reported by Li et al. (2008), with rye shoot N under predicted by 43% in 2005 and under predicted average annual N uptake of 1.2 kg N/ha or 2.5%. HERMES predicted the most N stress for winter rye in spring 2005. Although HERMES simulated crop biomass agreed reasonably well with observations in 2005, the simulated crop shoot N concentration and N uptake was under predicted that most likely indicates simulated N deficiency in soil. This argument would fit Section 3.1.6 below where HERMES is shown to over predict N loss in the fall of 2004 compared to field data, which would reduce simulated soil N availability in the fall and the following spring. Late fall 2004 measured total soil inorganic N levels were as high or higher than in other years (Kaspar et al., 2007), suggesting that fall N loss may have been over predicted by the model compared to field data. Thus, more N was available for the cover crop uptake than predicted by the model in spring 2005 and this coupled with good cover crop establishment and growth resulted in higher cover crop shoot N concentrations and N uptake than simulated.

3.1.3. Annual drainage

Average annual drainage was under predicted by 0.2 cm for NCC compared to field data (1%; EF = 0.69; RRMSE = 16%) and under predicted by 4.0 cm for CC (18%; EF = 0.11; RRMSE = 24%) (Table 4). The annual simulated drainage is within one standard deviation of observed for each year except for CC in 2002. Removing 2002, the EF is greater than 0.80 and the RRMSE <11% for both CC and NCC, which is similar to RZWQM drainage simulations reported by Li et al. (2008) when removing 2002 in the analysis. Drainage recorded as "observed" was in fact estimated for certain dates with missing data in 2002 possibly adding measurement error and contributing to HERMES under predicting drainage compared to "observed" (Li et al., 2008).

These results suggest the simple drainage component added to HERMES performed acceptably on an annual basis. The results discussed below suggest that the overall hydrology component and cumulative monthly simulated drainage performed acceptably for the objectives. Perhaps HERMES simulated drainage could be improved by adding a surface residue component as discussed below or simulating drainage using a slightly more detailed approach such as by Shen et al. (1998).

3.1.4. Monthly drainage

HERMES simulated monthly drain flow compared to observed data appears less accurate than RZWQM according to the figures of Li et al. (2008) even when 2002 data is removed from the analysis, mostly because HERMES over predicted flow in September through December 2003–2005 with an EF <0.5 for both CC and NCC (Fig. 2). HERMES may over predict drain flow late in the year because simulated soil evaporation does not account for surface residue, possibly resulting in over predicted drainable porosity to compensate for over predicted soil evaporation. In other words, the PEST program used to optimize the HERMES soil parameters including field capacity may have reduced the field capacity below field values resulting in more drainable porosity and less simulated stored soil water. This would increase HERMES simulated drain flow early in the season during peak flow when soil evaporation dominates ET and later in the season when the crop had matured and transpiration dominates ET to compensate on an annual basis for HERMES over predicted early season soil evaporation. The sensitivity analysis discussed below shows that decreasing field capacity increases HERMES simulated drainage. Shipitalo et al. (2015) reported that removing surface residue reduced RZWQM simulated subsurface drainage in northeastern Iowa from 16.5 cm/year to 9.4 cm/year because of increased soil evaporation. Thus future research should consider developing a surface residue component for the HERMES model, which may improve monthly drain flow simulations. The cumulative monthly drainage, however, is simulated very well by HERMES with EF >0.80 and within 20% of observed for both NCC and CC when including 2002: observed and simulated of 90.5 and 74.3 (CC) and 89.9 and 89.2 cm (NCC) (Fig. 2). Removing the 2002 data results in the cumulative monthly drainage simulated by HERMES within 10% for both NCC and CC: observed and simulated of 72.1 and 65.7 (CC) and 71.9 and 76.9 cm (NCC). In comparison, Branger et al. (2009) reported acceptable PESTDRAIN simulated cumulative drainage with EF >0.57 and drainage volume within 14% of observed. Li et al. (2008) did not quantify the performance of RZWQM for simulated monthly drain flow, however, the figures suggest that RZWQM did not over predict monthly drainage after August, and RZWQM reduces simulated ET as a function of increased surface residue.

In a comparable study, Bakhsh et al. (2000) used the GLEAMS model that, similar to HERMES, uses a tipping bucket (capacity) approach to simulate vertical water movement through soil (Wallis et al., 2011). Another similarity is that GLEAMS simulated percolate below the root zone was used to approximate drainage. The monthly GLEAMS simulated drain flow was not over predicted compared to field observed late season drainage in Iowa from chisel tilled plots. The no-till plots simulated by HERMES should have more surface residue than the chisel till plots of the GLEAMS study. Thus the effect of not considering surface residue on simulated evaporation from soil would be more pronounced with the current HERMES simulations. The correlation coefficients (R^2 values) were 0.51 and 0.57 setting the intercept to zero and comparing the GLEAMS simulated drainage to observed data. These may be similar or slightly better than the current central Iowa site (0.60 and 0.40; Fig. 3).

3.1.5. Simulated evapotranspiration

Average annual HERMES simulated ET from 2002 to 2005 for NCC and CC are 585 and 638 mm, which may be somewhat over predicted compared to field data partly due to lack of a surface residue component in HERMES as discussed above. In comparison, Sanford and Selnick (2012) reported average annual central Iowa ET to be about 500–600 mm between 1971 and 2000. Also, Thorp et al. (2007) reported 489 mm average annual RZWQM simulated ET between 2002 and 2005 for a different site in central Iowa, which they discuss as reasonable compared to regional measured annual ET. ET was not measured on the site simulated by Thorp et al. (2007) nor was it measured on the current site. Similar to our HERMES simulations, Li et al. (2008) reported 53 mm more RZWQM simulated ET with CC, mostly due to additional transpiration from the winter rye. Because of more HERMES simulated ET in CC compared to NCC, simulated drainage is 3.7 cm/year less in CC. In contrast to less HERMES simulated drainage on CC compared to NCC, 0.1 cm greater drainage was observed for CC (Table 4). It is difficult to determine if the HERMES simulated drainage difference between NCC and CC occurred on the plots (3.7 cm) because the average annual drainage standard deviation between replicates of both NCC and CC was fairly large (greater than 5 cm most years for both CC and NCC; Table 4).

3.1.6. Nitrate concentration

Average annual observed and HERMES simulated flow weighted nitrate concentration in drainage (FWNC) were 19.0 and 17.9 mg N/L for NCC and 7.2 and 9.5 mg N/L for CC, resulting in observed and simulated FWNC reductions due to cover crops of 62% and 47% (Table 4). In comparison, Li et al. (2008) showed a 49% reduction using RZWQM on the same fields and years. The EF <0 and RRMSE of 41% for CC suggests poor FWNC simulations by HERMES that are less accurate than Li et al. (2008) using RZWQM (Table 4). Two of the annual FWNC HERMES simulations outside the observed standard deviations are 2002 (CC) and 2005 (NCC). In 2002 observed and HERMES simulated FWNC were 4.3 and 9.0 mg N/L while the Li et al. (2008) RZWQM simulated CC concentration in 2002 was 5.0 mg N/L. The greatest monthly N loss simulated by HERMES in 2002 for CC was between April 1 and May 1 with 2.0 kg N/ha and 2.0 cm of drain flow (fig. 2). The average HERMES simulated N concentration in soil pore water for CC varied between 2 and 6 mg N/L between April 1 and May 1 at a depth of 0–90 cm (fig. 4). The HERMES simulated concentration was >10.0 mg N/L for most of this same time period at the drainage depth 110–120 cm (fig. 4). Therefore, part of the reason for the over predicted drainage N concentration in 2002 for CC may be that HERMES responds to some management differences and field conditions more slowly than RZWQM due to simulated full soil solution mixing of each soil layer. RZWQM simulates partial mixing and displacement of the soil solution which would tend to move soil solution in the surface layers more quickly to the drainage layer (Ahuja et al., 2000).

Relatively simple tipping bucket models for soil water and solute flow have included mobile and immobile phases. For example, the complex Richards equation based model LEACHP was simplified to a tipping bucket approach that included mobile and immobile water and soil solution solute transport (Hutson and Wagenet, 1993). Implementation of mobile and immobile phases could be

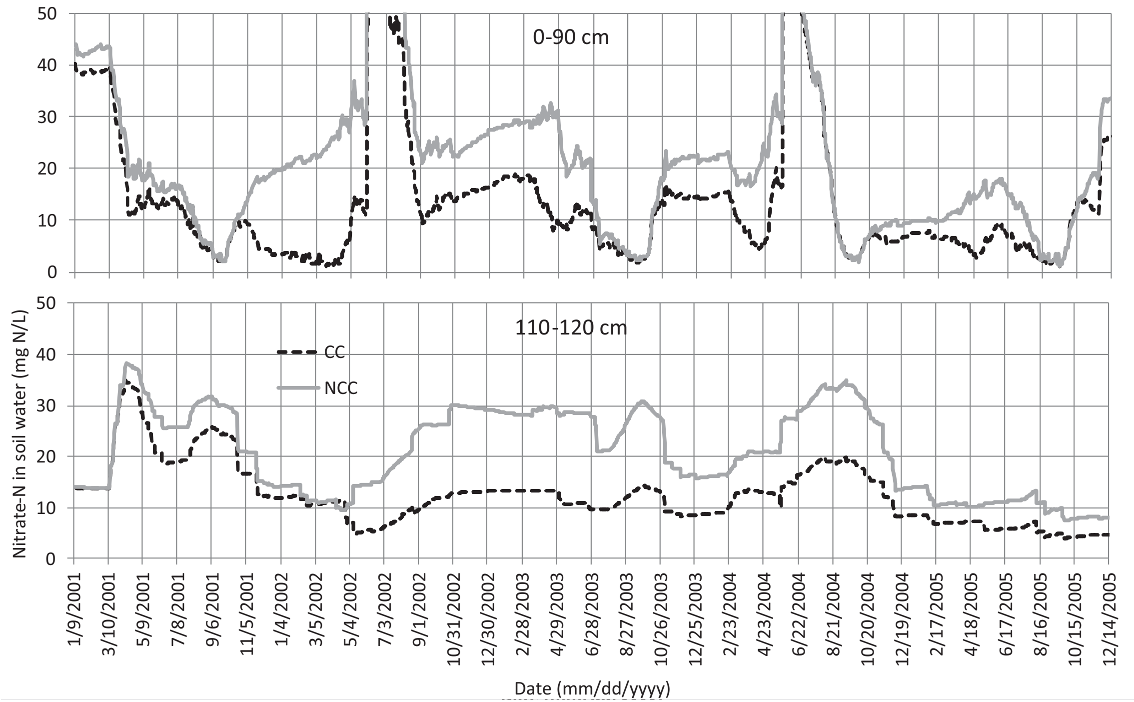

Fig. 4. HERMES simulated daily soil water nitrate-N concentration at two depth intervals (0–90 cm and 110–120 cm; mg N/L). CC is cover crop treatment; NCC is control treatment (no cover crop).

an approach to improve HERMES simulations for nitrate transport to subsurface drainage.

The least accurate HERMES simulated FWNC for NCC was in 2005 where observed and simulated concentrations were 18.5 and 10.9 mg N/L (Table 4). Part of this under predicted concentration could be because of over predicted N loss in late fall of 2004 (Fig. 2). The winter rye planted in fall of 2004 also showed the most HERMES simulated N stress in spring 2005 of all years and the largest under predicted rye shoot N was for spring of 2005, further suggesting that HERMES simulated soil nitrate was low in early 2005.

With the poor 2002 CC and 2005 NCC simulations, HERMES did not accurately simulate the year-to-year variability in annual FWNC differences between NCC and CC unlike RZWQM simulations reported by Li et al. (2008). Similar to Li et al. (2008) RZWQM simulations where overall FWNC difference between NCC and CC were under predicted by 3.7 mg N/L, HERMES under predicted overall FWNC differences by 3.3 mg N/L (Table 4). Li et al. (2008) discussed that RZWQM may have under predicted the FWNC difference because the cover crop in the field may have increased immobilization and reduced net mineralization (Parkin et al., 2006), which was not simulated. For our current HERMES simulation, the over predicted drainage and nitrate loss in the September thru December period may have increased the simulated FWNC of the cover crop treatment (CC) because nitrate was lost in the fall rather than spring and less time was allowed for N uptake by cover crop. Another possible contributing factor is that the CC plots may have greater observed field capacity than NCC plots as reported by Basche et al. (2016). The HERMES sensitivity analysis below suggests that greater field capacity results in reduced simulated annual FWNC. However, the field measurements of Basche et al. (2016) were taken in 2013, over 7 years after the simulated time period of 2002–2005, and the time period for the soil field capacity differences between CC and NCC is uncertain.

With a few poor FWNC simulations as discussed above, the EF values for annual FWNC were negative (Table 4), indicating that the average of FWNC measurements at the site were a better estimator of FWNC than HERMES. RZWQM also showed a negative EF for annual FWNC (NCC; Table 4). Li et al. (2008) discussed that other drainage model tests reported low EF values for annual FWNC such as Bakhsh et al. (2004) and Thorp et al. (2007). Although Youssef et al. (2006) discussed EF values associated with DRAINMOD simulations of monthly N loss, FWNC was not discussed.

3.2. Simulated N budget

The HERMES simulated annual nitrogen budget is shown in Table 5, which indicates that on average 25.5 kg N/ha less N is lost annually to drain flow from CC compared to NCC from 2002 through 2005. Most of this difference is due to 45.1 kg N/ha more N uptake by CC. Other important nitrogen budget components include 3.6 less N denitrification from CC, 17.0 more N mineralization from CC, 0.2 more N fixation from CC. The only remaining differences are the 3.5 kg/ha more N retained in the soil year to year from CC and 2.5 kg/ha more N leached to deep seepage from NCC (N lost to deep seepage not shown in Table 5). The simulated volatilization, application, and deposition of N are equal between CC and NCC.

Malone et al. (2015) listed one of the primary guidelines for model parameterization is to use "soft" data to optimize parameters, which can be interpreted in our case to mean that unmeasured model simulated values related to the nitrogen budget such as denitrification and mineralization should be reasonable for the field conditions. The average annual net mineralization for NCC was 132.0 kg N/ha, which appears reasonable but perhaps on the high side compared to seasonal totals (20 weeks) reported by Vigil et al. (2002) of up to 152 kg N/ha for 11 different field studies. Our annual mineralization rate is also slightly higher than 124.6 kg N/ha reported by Thorp et al. (2009) using DRAINMOD for central Iowa corn/soybean rotations. A very rough "rule of thumb" is about 35 kg of N per ha will mineralize in a twenty week season for every 1% of SOM in the soil (Vigil et al., 2002). The top 20 cm of our soil was 2.9% C or about 5% organic matter (SOM) assuming 1.72*soilC = SOM, suggesting seasonal mineralization could be as great as 175 kg N/ha.

Table 5
Simulated annual nitrate-N budget for winter rye cover crop (CC) and no cover crop (NCC) (all values in kg N/ha).[a]

Year	Fixation		Denitrification		Drain flow [b]		Total N uptake		Net mineral.		Annual soil N change	
	NCC	CC	NCC	CC	NCC	CC	NCC	CC	NCC	CC	NCC	CC
2002	0	0	22.7	18.6	17	8	294.5	322.5	131	142	34.9	32.7
2003	262[a]	260	13.9	10.3	82	29	344.9	403.5	128	143	−23.9	−12.2
2004	0	0	20.8	18.6	61	31	312.6	357.1	137	156	−30.6	−19.8
2005	241	244	13.5	8.9	18	8	340.2	390.8	132	155	50.6	44.3
Ave.	125.8	126.0	17.7	14.1	44.5	19.0	323.1	368.2	132.0	149.0	7.8	11.3
N budget for field capacity of 0.314 (see Tables 3 and 6)												
Ave.	127.8	128.0	29.7	23.4	35.5	13.8	322.8	367.1	132.0	149.3	8.3	11.2
Summary of Li et al. (2008) N budget												
Ave.	126.9	134.3	8.8	7.9	44.8	19.3	329.0	371.3	120.0	133.8	−2.7	1.8

[a] Annual HERMES N budget is presented to the significant digits provided in N budget output files.
[b] The drain flow N values differ slightly from Table 4 because HERMES drain flow is presented to the significant digits that are provided in specific HERMES drain flow output files; HERMES N budget output files provide less significant digits than the specific drain flow output files. Also, calculating monthly and annual values for Table 4 involved spanning January 1 because of sample collection dates, whereas the simulated-only Table 5 values do not span January 1. Synchronization of data with calendar year by interpolation or other means was not conducted because the effect is small.

HERMES simulated 17.7 kg N/ha average annual denitrification for NCC with an average annual fertilizer application and deposition of 146.0 kg N/ha, or denitrification was 12% of N applied. Meisinger and Randall (1991) reported that denitrification rates for a moderately well drained soil with 2% to 5% soil organic matter should range from 6% to 20% of N inputs from fertilizer and rainfall. In comparison, Thorp et al. (2009) simulated between 13 and 15 kg N/ha average annual denitrification using both RZWQM and DRAINMOD with an average of 106 kg N/ha fertilizer and deposition added per year. Parkin and Kaspar (2006) at an Iowa location close to the site simulated in our study measured average annual cumulative N_2O fluxes of 8.4 and 7.1 kg N_2O-N ha^{-1} for no-till corn-soybean rotations with and without a cereal rye cover crop, but dinitrogen flux associated with denitrification was not measured.

Average annual mineralization and denitrification for NCC are 12.0 and 8.9 kg N/ha greater with HERMES than RZWQM while total N uptake is 5.9 kg N/ha less for HERMES (Table 5). Fixation and N loss to drains are nearly equal between HERMES and RZWQM. The mineralization and denitrification differences could be because of the calibration of the two models and a slightly different calibration of each would result in less differences in the N budgets. For example, Li et al. (2008) used the RZWQM parameterization of Thorp et al. (2007) where denitrification and mineralization coefficients were calibrated to achieve acceptable model simulations of N loss and concentration in drain flow. For the HERMES calibration, we slightly reduced the fraction of organic matter that is available for slow decay from a default value of 0.13 to 0.12 to optimize model results (Table 3). Because of model equifinality (described in the next sentence), it's likely that slightly different calibrated parameter values would result in less difference between the HERMES and RZWQM simulated N budgets while providing acceptable simulations of the overall N dynamics. The equifinality concept suggests that many different model parameter sets within a chosen environmental model may be acceptable in reproducing the observed behavior of a system (Beven and Freer, 2001).

While the N budget comparison of a single treatment is important, the simulated N budget differences between the two treatments by HERMES and RZWQM are also important for our objectives. The NCC-CC N budget differences between HERMES and RZWQM are all within +−4 kg N/ha except HERMES simulates 0.2 kg N/ha more fixation for CC compared to NCC while RZWQM simulates 7.4 kg N/ha more fixation for CC. Both HERMES and RZWQM simulate fixation to meet N demand from soybean when demand exceeds soil availability. Table 5 also shows that both HERMES and RZWQM simulated slightly more denitrification from NCC compared to CC and about 14–17 kg N/ha more net mineralization. These NCC-CC denitrification differences are similar to a controlled laboratory study, where Parkin et al. (2006) reported lower N_2O emission from rye treatments than no rye under high manure application. But these HERMES and RZWQM denitrification simulations differ from a field study (Parkin and Kaspar, 2006) that showed slightly higher (but non-significant) N_2O emission with cover crops than without. Similar to the HERMES simulations, Constantin et al. (2012) reported more mineralization with catch crop treatments along with more N sequestered and less N leached.

3.3. Sensitivity analysis

The relative sensitivity coefficients (Sr) suggest that soil field capacity is the most sensitive variable tested affecting HERMES simulated N loss and flow weighted nitrate concentration in drainage (FWNC; Table 6). The Sr value of −1.4 (NCC) for field capacity essentially means that for each 1% increase in field capacity, FWNC decreases 1.4% for NCC. Table 5 shows that changing field capacity from 0.284 to 0.314 decreases HERMES simulated N loss to drain flow from 44.4 to 35.5 kg N/ha mostly because simulated denitrification increases from 17.7 to 29.7 kg N/ha. The increase in field capacity results in an increase in relative soil water saturation (RSWS) often called water filled pore space (soil water content divided by soil porosity), which is one of the main soil environmental variables driving HERMES simulated denitrification (Eq. (1); Kersebaum, 1995). For example under the increased compared to the original (or base) field capacity, the May 2004 simulated denitrification and surface 30 cm of soil water content increase as follows: simulated denitrification was 10.6 kg N/ha with an average soil water content of 0.303 cm/cm compared to denitrification of 6.3 kg N/ha with an average soil water content of 0.273 cm/cm. The large effect of a relatively small change in field capacity on HERMES simulated N loss to drain flow and denitrification is notable partly because Rawls et al. (1982) lists the range of field capacity for clay loam soil of 0.25–0.39 (Table 3). The sensitivity to field capacity is also notable because Basche et al. (2016) recently reported significantly greater field capacity measured in the cover crop plots (CC) compared to NCC of the current field site in Boone County Iowa. A greater field capacity input for CC compared to NCC results in lower HERMES simulated FWNC in CC (Table 6), which would reduce or eliminate the observed and simulated FWNC difference (Table 4).

Both Breve et al. (1997) and El-Sadek and Vazquez (2012) report that DRAINMOD-N predictions of nitrate in drainage were sensitive to the denitrification coefficient. David et al. (2009) studied several models that could estimate N loss to subsurface drainage along with denitrification and noted that the simulated denitrification by the hydrologic model SWAT is sensitive to field capacity. Marchetti et al. (1997) investigated a number of crop models and found that

Table 6
Sensitivity analysis.

HERMES output	Field capacity		Porosity		Wilting point		Fraction of organic matter that is available for slow decay		Drainage fraction		AMAXC	
	Parameter change from base value (%) [dP is in brackets]											
	(10.6%) [3.0 cm/cm]		(9.5%) [4.0 cm/cm]		(13.8%) [2.0 cm/cm]		(8.3%) [0.01 kg/kg]		(6.7%) [0.005]		(9.5%) [8.0]	
	NCC	CC	NCC	CC	NCC	CC	NCC	CC	NCC	CC	NCC	CC
	Average annual HERMES output with increased parameter value (P + dP)											
N loss	35.4	13.8	47.3	20.8	44.1	18.7	44.8	19.2	46.2	19.4	41.7	16.7
drain flow	21.4	17.6	22.3	18.6	22.6	19.0	22.3	18.6	23.8	19.8	22.2	18.5
FWNC	14.9	7.5	19.1	10.4	17.6	9.2	18.1	9.6	17.5	9.0	17.0	8.5
Average annual HERMES output with decreased parameter value (P − dP)												
N loss	51.3	23.7	40.0	16.4	44.3	19.0	44.0	18.6	42.2	18.2	47.8	22.1
drain flow	23.3	19.7	22.3	18.6	21.7	17.9	22.3	18.6	20.8	17.3	22.1	18.4
FWNC	20.3	11.3	16.2	8.3	18.4	9.9	17.8	9.3	18.3	9.8	19.5	11.1
Relative sensitivity coefficients (Sr)												
N loss	−1.7	−2.5	0.9	1.3	0.0	−0.1	0.1	0.2	0.7	0.5	−0.7	−1.5
drain flow	−0.4	−0.5	0.0	0.0	0.2	0.2	0.0	0.0	1.0	1.0	0.0	0.0
FWNC	−1.4	−1.9	0.9	1.3	−0.3	−0.3	0.1	0.2	−0.4	−0.6	−0.7	−0.7

All HERMES output is average annual: N loss to drain flow, drain flow volume, and flow weighted nitrate concentration (FWNC). The dP is the difference between the base parameter value (P) from Table 3 and the adjusted parameter value.

simulated denitrification was sensitive to field capacity. In contrast to the current HERMES results, the figures of Marchetti et al. (1997) suggest that CERES-N and GLEAMS simulated a decrease in denitrification with an increase in field capacity suggesting variability of simulated denitrification among models. Other investigations have noted the variability of simulated denitrification among agroecosystem models. Remarking on this variability, David et al. (2009) concluded "model comparisons suggest our ability to accurately predict denitrification fluxes (without known values) from the dominant agroecosystem in the midwestern Illinois is quite uncertain at this time." Despite some related studies as discussed here, few articles appear to fully address the sensitivity of simulated nitrate concentration in subsurface drainage and the associated sensitivity of simulated denitrification to changes in soil field capacity. Related lab and field studies also appear limited. Castellano et al. (2010) stated "As far as we know, the relationship between N_2O flux and matric potential has not been previously examined across soil types and water contents." Using soil columns collected from three landscape positions, Castellano et al. (2010) reported maximum N_2O flux rates occurred at approximately field capacity and concluded that matric potential is the strongest predictor of the timing of N_2O flux across soils that differ in texture, structure and bulk density. Van der Weerden et al. (2012) also found that matric potential was the best estimator of N_2O emissions from different soils, but they concluded that the second best property explaining N_2O emissions, volumetric soil water content, is more readily determined than matric potential and may be a more appropriate estimator. In a synthesis of 20 years of experimentation, Ball (2013) noted that soil matric potential is a relevant indicator for N_2O flux and concluded that "pore-scale models are likely to have an increasing role in understanding mechanisms of greenhouse gas production". In our current study, increasing field capacity by about 11% (Table 6) results in HEMES simulated denitrification rates to increase about 70% (Table 5) and nitrate concentrations in drainage (FWNC) to decrease about 17% (Tables 4 and 6). Investigative modeling approaches are part of the intrinsic value of biogeochemical models (Oreskes et al., 1994). Here we determine that in accordance with related research (Castellano et al., 2010; David et al., 2009; Marchetti et al., 1997), soil field capacity is a critical parameter to investigate to more thoroughly understand and appropriately model denitrification and N loss to subsurface drainage.

Of course with the sensitivity of HERMES simulated denitrification to simulated water filled pore space, soil porosity was a sensitive variable affecting N loss with Sr values of 1.3 (CC) and 0.9 (NCC) (Table 6). Another sensitive variable tested was the corn growth coefficient AMAXC (Table 3) with Sr values of −1.5 (CC) and −0.7 (NCC) for N loss and −0.7 (CC) and −0.7 (NCC) for FWNC (Table 6). Increasing the AMAXC from 83.8 to 91.8 kg CO_2/ha leaf/hour resulted in HERMES simulated N loss to drainage to decrease from 46.0 to 41.7 kg N/ha (). Much of this decrease was because the corn yield increased a relatively small amount from 10.5 to 10.9 Mg/ha in 2002 with a total N uptake increase by the corn from 246 to 257 kg N/ha. The HERMES simulated N uptake by corn did not change as much in 2003 (from 275 to 278 kg N/ha). Malone and Ma (2009) reported that relatively small increases in RZWQM simulated N uptake by crops (about 3% for the two years of corn in our case) can result in relatively larger decreases in RZWQM simulated N loss to drainage (about 9% over the four year period in our case).

4. Summary and conclusions

These results and analysis: 1) suggest that HERMES shows potential to simulate the effects of winter rye on reducing N loss to subsurface drainage when compared to four years of measured data and 2) identified important input parameters to closely examine. The less accurate simulations and related discussion (e.g., fall drainage most years and FWNC for CC in 2002) helped identify HERMES modifications that could improve simulations of N loss to subsurface drainage. The HERMES simulated annual and cumulative drainage were reasonable compared to observed data, similar to the more complex RZWQM simulations, and similar to other model drainage tests reported in the literature. Although the annual N loss simulations by HERMES were reasonable for the most part, the model did not accurately simulate the variability in 1) year-to-year annual nitrate concentration in drainage (which has been reported for other published drainage model tests as well) nor 2) annual NCC-CC nitrate concentration differences. HERMES did not simulate the annual NCC-CC nitrate concentration differences as accurately as RZWQM, possibly because RZWQM simulates partial mixing and displacement of the soil solution and RZWQM simulates reduced soil evaporation when surface residue is present. HERMES does not simulate these two processes. The N budget analysis suggests that the unmeasured simulated components are within published ranges for the site conditions, such as annual denitrification and net mineralization. Both the current HERMES simulations and the previous RZWQM simulations of Li et al. (2008) under predicted the effect of winter rye in reducing N concentration in drainage. The results of this study and recent field research on the site suggests that this under prediction could be partially due to greater soil field capacity on CC. Field capacity was found to be the most sensitive HERMES parameter investigated affecting N loss to drainage, with increased field capacity resulting in increased HERMES simulated denitrification and increased soil water content along with reduced nitrate concentration in drain flow.

Anthropogenic perturbation of the global nitrogen cycle and its effects on the environment such as hypoxia in coastal regions is of increasing, cross-disciplinary, worldwide concern, and food production is the major contributor (Galloway et al., 2003; Gruber and Galloway 2008; Canfield et al., 2010). Field research has shown that a fall-planted "winter" cover crop is an agricultural management practice that reduces nitrate losses from artificially drained agricultural fields (e.g., Kaspar et al., 2012) and modeling research suggest adding winter rye as a cover crop could help reduce the hypoxic zone in the Gulf of Mexico and elsewhere if implemented on a large scale (Malone et al., 2014a; Kladivko et al., 2014). Our results suggest that the relatively simple HERMES model modified to simulate subsurface drainage is a promising tool to help evaluate the effects of management practices such as winter cover crops on N loss to drainage. Our results also suggest that soil field capacity is a critical parameter to investigate to more thoroughly understand and appropriately model denitrification and N loss to subsurface drainage, which is a research area where lab and field studies are limited (Castellano et al., 2010).

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