Available online at www.sciencedirect.com
ScienceDirect
Computers and Electronics in Agriculture 53 (2006) 113–121
Computers and electronics in agriculture
www.elsevier.com/locate/compag

Fate and transport of nitrogen compounds in a cold region soil using DRAINMOD

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Received 22 August 2005; received in revised form 7 April 2006; accepted 29 April 2006

Abstract

Freezing and thawing cycles in soil can have a significant effect on field hydrology, which, in turn, can have a major influence on the fate and transport of agricultural chemicals. This study was conducted to evaluate the hydrological performance and NO_3^--N movement of the DRAINMOD 5.1 model with respect to freezing/thawing conditions. Measurements made in the years 1999 and 2000 at an experimental site in Truro, Nova Scotia, Canada on four test plots receiving inorganic fertilizer were used to test the model. Monthly subsurface drainage outflows, simulated using the original and DRAINMOD 5.1, were compared with the observed values. The results showed that the original DRAINMOD overestimated drain outflows during the colder months. The average difference between the monthly drainage outflows, simulated with DRAINMOD 5.1, and the observed values ranged from −0.35 to −1.42 mm. Since the new model predicted the timing and magnitude of drainage events quite well and also did a much better job of simulating the hydrology of a colder region, as compared to the original model, it was used to simulate fate and transport of nitrogen compounds. The model was calibrated with the data from two test plots, and validated with the data from the remaining two plots. The difference between the simulated and observed total NO_3^--N losses over a period of 2 years were, respectively, 1.32 and 1.40 kg N/ha for the calibration plots. For validation plots, they were −1.64 and 0.97 kg N/ha, respectively. These results indicate that the DRAINMOD 5.1 model, performed satisfactorily, and may be used to estimate NO_3^--N losses through drainage outflow in colder regions.

Keywords: DRAINMOD; DRAINMOD-N; DRAINMOD 5.1; Subsurface drainage; Freezing-thawing; NO_3^--N losses

1. Introduction

The climate in Atlantic Canada is characterized by a cool and moist spring and fall, dry summer, and cold winter in which freezing, thawing, and snow melt often occur. The snow melting process and the daily freezing-thawing cycles can have a dominant effect on the overall field of hydrology. Frozen soil surface layers often result in no or

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0168-1699/$ – see front matter
doi:10.1016/j.compag.2006.04.005

low infiltration rates, and surface runoff can occur as a result of rainfall and snowmelt (Zuzel et al., 1982; Johnsson and Lundin, 1991). Occasionally, snowmelt can be large enough to cause both surface and subsurface drainage to occur, and this can have an important bearing on the solute transport and regional water quality (Stahli et al., 1999). Therefore, effective evaluation of field hydrology and chemical transport in soils of cold regions is of particular practical importance in agricultural water management.

Currently, several computer simulation models are available that can simulate the flow process and chemical transport through soil profiles and into sub-surface drainage systems. However, only a few of these models can effectively simulate the dynamics of heat and water flow in soils subjected to freezing and thawing cycles (Stahli et al., 1999). The field hydrological model, DRAINMOD (Skaggs, 1978), has been used successfully to simulate surface and subsurface drainage discharges and fluctuations in midspan water tables for a wide range of soils, crops, weather conditions, and water management practices; however, this version did not incorporate freezing and thawing (Skaggs, 1982; Fouss et al., 1987; Cox et al., 1994; Shukla et al., 1994).

Using the hydrological simulations of DRAINMOD, Brevé et al. (1997a,b) extended the model to estimate nitrogen movement in agricultural soils by developing DRAINMOD-N. Zhao et al. (2000) also applied this model for predicting nitrogen losses in drainage water in a well-drained clay loam soil in Minnesota. Although they successfully simulated nitrate losses, freezing and thawing was not considered in their study, and the simulations were limited to April to August. Singh et al. (2001) also successfully predicted nitrate losses using the model for poorly drained soil in Central Illinois; however, they too used DRAINMOD-N, not DRAINMOD 5.1.

Recently, DRAINMOD-N has been incorporated into version 5.1 of DRAINMOD, which also includes a freezing and thawing component for colder climates (http://www.bae.ncsu.edu/soil_water/drainmod.htm; Sands et al., 2003). The new model calculates the daily average soil temperature profile, considers the effect of ice formation on soil hydraulic conductivities and infiltration capacity based on average ice content in the frozen layer. A rain/snow-dividing base temperature is used to identify the precipitation as rain or snow. The details of the new algorithm and associated modifications were presented by Luo et al. (2000). The new model showed improvement in prediction of hydrology in colder climates (Luo et al., 2001; Sands et al., 2003).

In this study, DRAINMOD 5.1 version is used for simulating both soil hydrology and NO_3^--N movement. The objective of this study was to (1) test the hydrologic performance of the DRAINMOD 5.1 model for a cold region in Atlantic Canada, and (2) compare the simulated and observed NO_3^--N losses in subsurface drains. To the best of our knowledge, fate and transport of NO_3^--N in a cold region using DRANMOD 5.1 has not been published before.

2. Materials and methods

2.1. Experimental site

The experimental site was located at the Atlantic Agri-Tech Park of the Nova Scotia Agricultural College in Truro, Nova Scotia, Canada (45°22′N 63°16′W). It consists of eight subsurface drainage plots, each 24 m wide by 48 m long, with an area of 1152 m^2. Each plot contained two 100 mm diameter tile drains. Drains were installed at 0.80 m depth with 12 m spacing. Experimental plots were isolated by buffer drains to prevent lateral water movement between the plots. The drain outflows from each plot flowed directly into a water sampling room in the adjacent facility. Hourly flow rates were continuously recorded using tipping buckets, which were wired to a Campbell Scientific CR10X data logger. Water samples for NO_3^--N analysis was collected from flowing water discharging from the tipping buckets. Sampling was performed according to a flow-weighted average strategy, in which the frequency of water sampling was set according to accumulated drainage volume. This strategy was adopted to ensure that samples were collected throughout the entire flow event. Water samples were collected manually in 50 ml Fisher Scientific Falcon Blue bottles and immediately frozen and stored, prior to transport to the Charlottetown Research Station of Agriculture and Agri-Food Canada in Prince Edward Island for analysis. The midspan water table fluctuations and the surface runoff were not observed, thus, the comparison between observed and simulated values was limited to subsurface drainage.

2.2. Soil properties

There were three types of soil groups at the experimental site, namely, Pugwash82, Pugwash52, and Debert22. Pugwash52 (plots 4, 5, 6) and Pugwash82 (plots 1, 2, 7) soils covered approximately 75% of the site, and were moderately well-drained with a friable, fine sandy loam-textured Ap horizon, 25 cm thick, underlain by a friable, 15–20 cm thick, fine sandy loam-textured Bm horizon. Below the Bm horizon was a friable-to-firm, fine sandy loam-textured BC horizon, grading into a weakly structured, friable, fine sandy loam-textured C horizon. The remaining 25% of the field was an imperfectly drained Debert22 soil (plots 3, 8), with a friable, 25–30 cm thick, sandy loam-textured Ap horizon, underlain by a friable, 25–30 cm thick, sandy loam-textured Bm horizon. The Bm horizon overlaid poorly structured subsoil horizons that usually start between 40 and 70 cm from the surface. Due to a high water table in this region, artificial drainage is necessary to crop growth.

2.3. Agronomic practices

Field experiments were conducted in 1999 and 2000, in which liquid hog manure was applied to plots 1, 3, 5, and 7, and the inorganic fertilizer to plots 2, 4, 6, and 8. Crops grown in the field were barley in 1999 and carrots in 2000. Barley was planted on 17 May 1999 and harvested on 24 August 1999. Carrots were seeded at a rate of 40 seed m^{-1} on 22 May 2000 and harvested on 8 October 2000. The plots receiving inorganic fertilizer used a 17-17-17 fertilizer blend in 1999 and 12-24-22 in 2000 at a conventional rate of 70 kg N ha^{-1} in the beginning of crop planting. Carrots in 2000 were fertilized again with ammonium nitrate at the rate of 168 kg ha^{-1} on July 25th. Buffers between the plots had no fertilizer applied in either year. In this study, only the plots receiving the inorganic fertilizer were used to evaluate the model.

3. Model inputs

Daily minimum and maximum temperatures are used to calculate the potential evapotranspiration in DRAINMOD using the Thornthwaite method (Skaggs, 1978). The observed daily rainfall values were converted to hourly values with the help of a subroutine in the DRAINMOD 5.1 package, assuming that the daily rainfall was uniformly spread over 4 h.

The soil water retention characteristics were obtained using the standard pressure plate method for each horizon of the three soil groups. The drained volume and upward flux for a specified water table depth were calculated by DRAINMOD. The saturated hydraulic conductivities (K_{sat}) were determined by the core method (Klute and Dirksen, 1986). The physical property inputs of three soil groups for different soil layers are shown in Table 1.

In order to reflect the freezing and thawing phenomenon, additional inputs were required (Luo et al., 2000), including the two constants relating soil thermal conductivity to soil water content, the rain/snow-dividing temperature, the snow melt base temperature and degree–day coefficient for snowmelt, the critical ice content above which infiltration stops, the initial soil temperature distribution and a base temperature as the lower boundary condition, the phase lag for daily

Table 1
Soil physical properties

Soil type	Plot no.	Depth (cm)	K_{sat} (mm/day)	Volumetric soil moisture retention (%) at different pressure heads						
				0 kPa	5 kPa	10 kPa	33 kPa	100 kPa	300 kPa	1500 kPa
Pugwash82	2	0–25	480	46.4	38.3	37.3	34.9	33.0	16.8	11.1
		25–44	240	35.8	30.8	29.6	27.6	25.6	16.6	11.5
		44–76	168	35.6	30.8	29.3	27.2	25.6	16.1	10.8
		76–100	120	34.3	29.4	27.1	24.3	21.7	11.6	7.7
Pugwash52	4 and 6	0–25	480	53.5	42.8	41.2	38.4	35.6	15.2	12.6
		25–44	216	34.5	29.4	28.5	26.1	23.3	16.8	11.3
		44–76	144	34.0	29.0	28.4	26.6	24.8	17.7	11.2
		76–100	96	36.1	27.6	25.1	22.7	20.7	15.5	8.3
Debert22	8	0–24	480	50.0	39.1	38.3	35.3	31.3	15.1	9.4
		24–38	192	33.1	27.2	26.7	24.7	20.9	17.0	11.3
		38–80	120	35.3	31.6	31.2	28.4	24.8	17.3	13.5
		80–100	96	38.4	33.0	32.1	28.3	23.0	18.9	11.7

Table 2
DRAINMOD input parameters

Parameters	Value	Units
Drainage system		
Drain depth	0.8	m
Drain spacing	12	m
Effective radius	5.0	mm
Depth from drain to impermeable layer	1.0	m
Soil temperature		
Thermal conductivity function coefficients	$a = 0.553$, $b = 1.963$	W/m °C
Diurnal phase lag of air temperature	9	h
Base temperature as the lower boundary	7	°C
Rain/snow dividing temperature	0	°C
Snowmelt base temperature	1.5	°C
Degree–day coefficient	5	mm/day
Critical ice content	0.2	cm^3/cm^3
Nitrogen dynamics		
Net mineralization rate (K_{min})	3×10^{-5}	1/day
Denitrification rate (K_{den})	0.3	1/day
Dispersivity (λ)	0.05	m
NO_3^--N concentration from rain	1.0	mg/l

air temperature sine wave, the initial snow depth and density, and soil freezing characteristics which indicates the relationship between unfrozen water content, and soil temperature. Kuz'min (1961) suggested 2 °C for snowmelt base temperature on typical topography of the plains; snow would begin to melt when the average air temperature exceeded 2 °C. The snowmelt degree–day coefficient is generally about 5 mm/°C day (Kuz'min, 1961). The critical ice content to block infiltration depends on soil conditions, but it can be estimated as 60% of the field capacity or 60% of the volumetric soil water content corresponding to a pressure head of about −300 cm. When the ice content exceeds this critical value, infiltration ceases and snowmelt leaves the surface as runoff. The lower boundary was assumed to be a constant soil temperature, which can be approximated as the long-term average air temperature (Penrod et al., 1958). The values of the above-mentioned parameters are used in this study, and are listed in Table 2.

The nitrogen-related parameters were the standard rate coefficients for denitrification (K_{den}) and net mineralization (K_{min}), the soil dispersivity (λ), and the nitrogen content in the rain and crops. Based on a range reported in the literature (Brevé et al., 1997a), K_{den}, K_{min} and λ were obtained by comparing the simulated and observed drainage NO_3^--N losses that resulted in the best agreement using data from Pugwash52 field (plots 4 and 6). These calibrated values were used as input in nitrogen simulation of the other two plots. The nitrogen content in barley and carrot was based on the observed data. The main parameters required in the model are also summarized in Table 2.

4. Methods of evaluation

The model was evaluated using both graphical and statistical methods. In the graphical approach, the hydrological simulations, with both the original and DRAINMOD 5.1 models, for the 2 years are compared with the observed values. Also, the simulated monthly and cumulative NO_3^--N losses via subsurface drainage simulated with DRAINMOD 5.1 are compared with the observed data. The model performance was quantified by calculating the following statistical parameters: average mean of the difference (MD), the mean absolute error (MAE), the modeling efficiency (EF), and the coefficient of determination (R^2), as shown below (Loague and Richard, 1991):

$$\mathrm{MD} = \frac{1}{n}\sum_{i=1}^{n}(O_i - P_i) \quad (1)$$

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}|O_i - P_i| \quad (2)$$

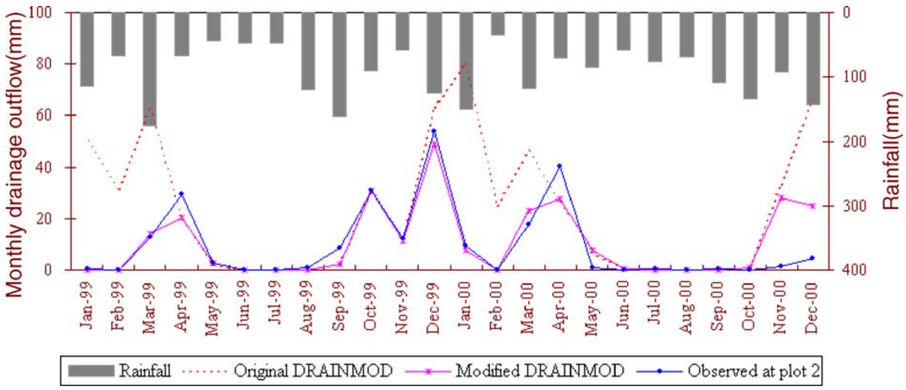

Fig. 1. Simulated vs. observed monthly drainage outflows at plot 2.

$$\mathrm{EF} = \frac{\sum_{i=1}^{n}(O_i - \bar{O})^2 - \sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \tag{3}$$

$$R^2 = \frac{\left(\sum_{i=1}^{n}(O_i - \bar{O})(P_i - \bar{P})\right)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2 \sum_{i=1}^{n}(P_i - \bar{P})^2} \tag{4}$$

where O_i is the observed value at time i, P_i the predicted value at time i, $\bar{O}$ the mean of the observed values over the time period (1 to n), and $\bar{P}$ is the mean of the predicted values over the time period (1 to n). The MD gives information on whether a model is under- or over-estimating. MAE is an indicator of the quantitative dispersion between the predicted and observed values, and EF compares how the predicted values are better than the average value of the measurements. The R^2 is the square of the Pearson's product-moment correlation coefficient, describing the agreement between the predicted and observed values. Ideally, the values of MD and MAE should be zero and the values of EF and R^2 equal to 1. If EF is less than zero, the model-predicted values are worse than simply using the observed mean (Loague and Richard, 1991).

5. Results and discussion

5.1. Hydrologic simulation

The predicted and observed monthly subsurface drainage outflows at plots 2, 4 and 6, and 8 in 1999 and 2000 are compared in Figs. 1–3, respectively. In these figures, simulations using both the original and DRAINMOD 5.1 are presented. It is evident from the figures that the new model performed better than the original DRAINMOD during the

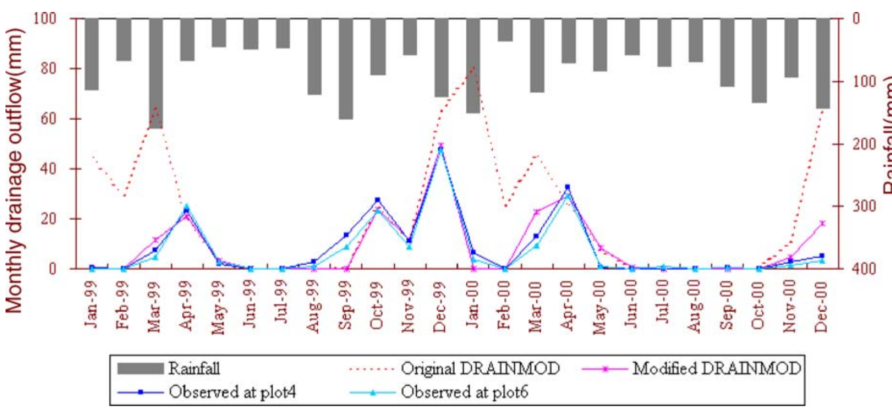

Fig. 2. Simulated vs. observed monthly drainage outflows at plots 4 and 6.

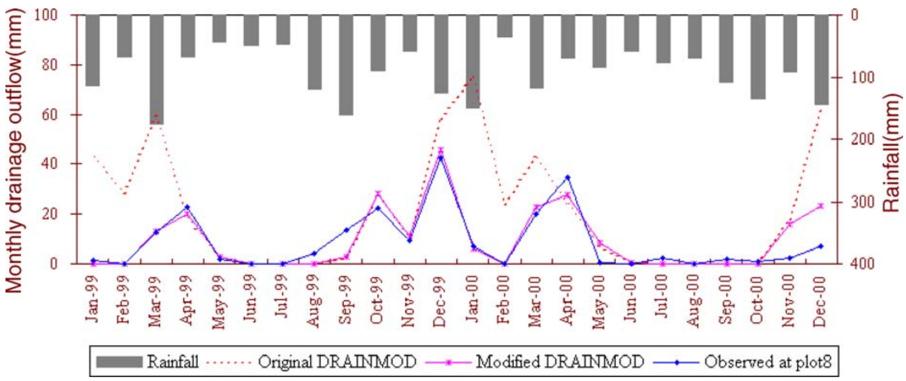

Fig. 3. Simulated vs. observed monthly drainage outflows at plot 8.

winter season. The original model overestimated the drainage outflows in the winter. The new model separated rain and snow, and kept snow on the ground until the average air temperature rose above the snowmelt temperature, thus, correcting the timing and magnitude of drainage response to snow.

The largest differences between the predicted and observed monthly drainage for the new model occurred in November and December of 2000. During this period, there was more rainfall, but less observed drainage. The model seems to be more responsive to rainfall than what the observed data would indicate. However, during all other periods, the predicted monthly drainage outflows were in good agreement with the observed values. It should also be noted that deviation from observed values was lower in the case of DRANMOD 5.1 as compared to that with the original model.

The total rainfall was 1114 mm in 1999 and 1136 mm in 2000, and the monthly rainfall distribution was similar during the 2 years of simulation. However, the total observed drainage outflows in 1999 were greater than that in 2000. In 1999, there were 11 days having rainfall greater than 25 mm, totaling 374 mm of rain, whereas in 2000, the number of such days was only 5, which caused only 176 mm of rain. Thus, heavy rainfall occurred more often in 1999 as compared to 2000. It was also observed that intense rainfalls occurred after certain preceding rainfall events in 1999. In 2000, the rainfall was generally well distributed. So, more runoff was caused in 1999. Average precipitation of the region is 1202 mm, thus, rainfall amount in both the years can be considered to be typical in terms of the total rainfall.

The statistical indices calculated from the predicted and observed monthly drainage outflows using original and DRAINMOD 5.1 are shown in Table 3. The indices for the four plots are comparable to each other. The MD for original DRAINMOD ranged from −12.23 to −14.37 mm, which indicated that the model slightly overestimated drain flow. The corresponding values for the new model ranged from −0.35 to −1.42 mm, which indicated that there was negligible error in simulated drain flow, and there was no under- or over-estimation of drain flow. The MAE for the new model ranged from 3.00 to 4.17 mm, as compared to 15.18 to 16.63 mm for the original model, which again established a good model performance. The EF values ranged from 70% to 83% for the new model, whereas the same for original model were from −443% to −251%. This showed that the new model simulated drain flow much more accurately than the original DRAINMOD model that gave negative EF values. The R^2 for each plot was higher than 0.8, once again showing that the simulated and observed values were in good agreement. Thus, the statistical indices clearly

Table 3
Statistics of simulated and observed monthly drainage outflows for 1999 and 2000 using the original and new DRAINMOD model

Model	Site	MD (mm)	MAE (MM)	EF (%)	R^2
Original	Plot 2	−13.79	16.63	−251	0.17
	Plot 4	−13.30	15.82	−370	0.15
	Plot 6	−14.37	16.11	−443	0.12
	Plot 8	−12.23	15.18	−340	0.19
New	Plot 2	−1.01	4.17	70	0.70
	Plot 4	−0.35	3.07	83	0.84
	Plot 6	−1.42	3.00	81	0.84
	Plot 8	−0.83	3.60	76	0.79

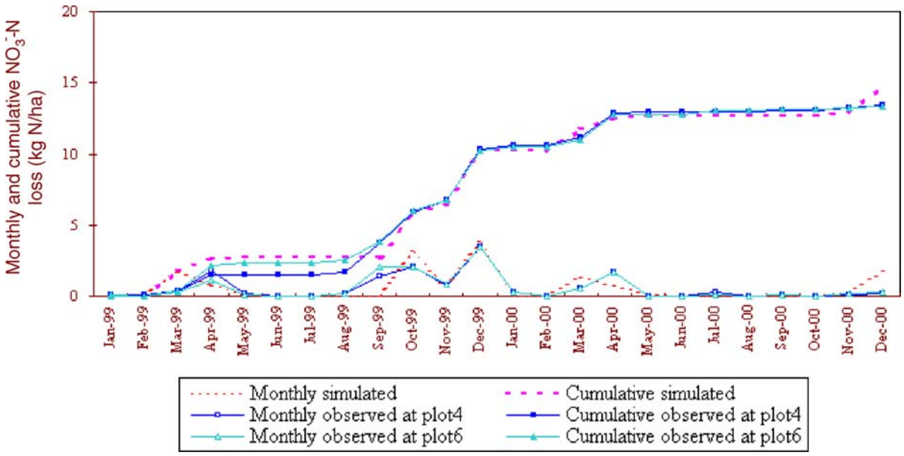

Fig. 4. Simulated vs. observed monthly and cumulative $NO_3{}^{-}$-N losses in subsurface drainage at plots 4 and 6.

show that DRAINMOD 5.1, which incorporates freezing and thawing, can simulate subsurface drainage outflows in a satisfactory way in colder regions.

5.2. Nitrogen simulation

A set of nitrogen simulations was conducted to calibrate the nitrogen component of model DRAINMOD 5.1 using data from Pugwash52 (plots 4 and 6). The main parameters, K_{den}, K_{min} and λ (see Section 3), were calibrated based on the best agreement between the predicted and observed $NO_3{}^{-}$-N losses in subsurface drainage on the basis of the values of statistical parameters. The calibrated values were used as input in the nitrogen simulations of the other two plots. The initial nitrate distribution in the soil profile, initial organic nitrogen and other parameters were assumed to be the same for all four plots.

The results of monthly and cumulative $NO_3{}^{-}$-N losses in subsurface drainage for plots 4 and 6, 2, and 8 are shown in Figs. 4–6, respectively. The statistical indices, calculated for the predicted and observed monthly $NO_3{}^{-}$-N losses, are shown in Table 4. It appears from Fig. 4 that the calibration for plots 4 and 6 is satisfactory, and the cumulative predicted $NO_3{}^{-}$-N losses are in good agreement with the observed values. Following the over-estimated drainage outflows, DRAINMOD 5.1 slightly overestimated the monthly losses in March of both years. The MD of $NO_3{}^{-}$-N losses was −0.055 and −0.058 kg N/ha, thus, the difference between simulated and observed over a 2-year period was only 1.32 kg N/ha for plot 4 and 1.4 kg N/ha for plot 6. Therefore, it can be stated that there was no under- or over-estimations. The MAE was 0.40 kg N/ha for both these plots, and the error between predicted and observed $NO_3{}^{-}$-N

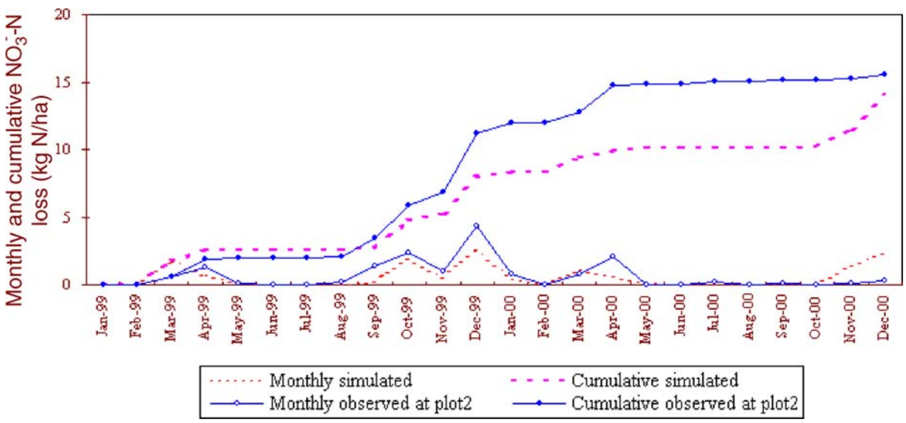

Fig. 5. Simulated vs. observed monthly and cumulative $NO_3{}^{-}$-N losses in subsurface drainage at plot 2.

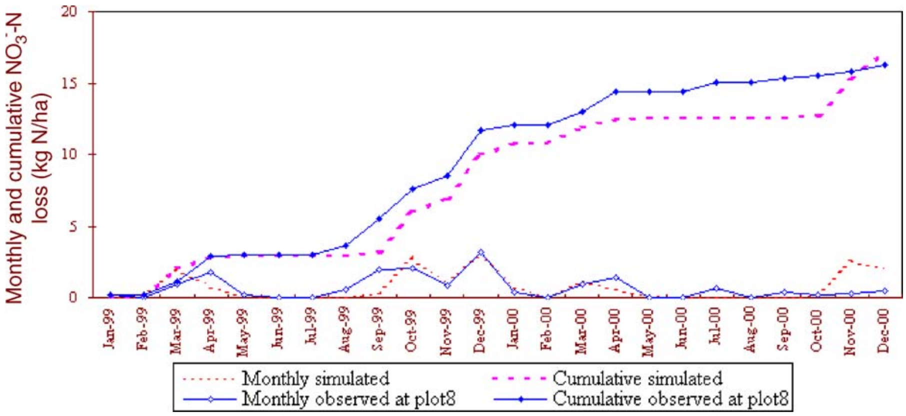

Fig. 6. Simulated vs. observed monthly and cumulative NO_3^--N losses in subsurface drainage at plot 8.

Table 4
Statistics of simulated and observed monthly NO_3^--N losses for 1999 and 2000

Site	MD (kg N/ha)	MAE (kg N/ha)	EF (%)	R^2
Plot 2	0.068	0.49	39	0.43
Plot 4	−0.055	0.40	39	0.55
Plot 6	−0.058	0.40	42	0.59
Plot 8	−0.040	0.50	07	0.40

was reasonable. The R^2 values were higher than 0.70. Thus, the model calibration was satisfactory. The EF values were not very impressive due to their sensitivity to a few large errors, especially in smaller data sets.

The validation results for plots 2 and 8 showed that the predicted monthly NO_3^--N losses were similar to plots 4 and 8 (Figs. 5 and 6). In plot 2, there was slight under-estimation in December 1999 and April 2000, which was reflected in lower simulated cumulative losses. Similarly, in plot 8, there was slight under-estimation for September 1999. Nevertheless the statistical parameters, i.e. MD, MAE, and R^2, for both plots were comparable to those for the calibration plots (Table 4). The differences between the predicted and observed total losses over the 2-year period were −1.64 and 0.97 kg N/ha for plots 2 and 8, respectively. So, we can conclude that DRAINMOD 5.1 performed well at simulating nitrogen losses via subsurface drainage in Atlantic Canada.

6. Conclusions

With the release of DRANMOD 5.1, the model has been modified recently to include freezing, thawing and snowmelt components, and has also been extended to include movement and fate of nitrogen. This study was conducted to verify the improvement in drainage outflow simulations with the new DRAINMOD model, and to test its nitrogen simulation capability in a cold region. The data used to validate the model was collected in Truro, Nova Scotia, Canada, over a 2-year period. The simulated monthly drainage outflows by the original and new DRAINMOD were compared with the observed values. The original DRAINMOD over-estimated drainage outflow during the colder months (December to April). However, the results showed that the new model satisfactorily predicted the timing and magnitude of drainage events. The observed and predicted drain outflows were comparable to each other.

For NO_3^--N simulations, the model was first calibrated with the data from two test plots, and then validated with the data from the remaining two plots. The difference between the simulated observed total NO_3^--N losses over the 2-year period were 1.32 and 1.40 kg N/ha for the calibration plots. The results for the validation plots were comparable with the calibration results, and the difference between the simulated and observed NO_3^--N losses were −1.64 and 0.97 kg N/ha in the 2 years. Thus, the performance of DRAINMOD 5.1 was deemed satisfactory. It may be concluded that DRAINMOD 5.1 model can be used to simulate drainage outflows and NO_3^--N losses through drain outflows in cold regions.

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