Understanding soil nitrogen processes in diversified vegetable systems through agroecosystem modelling

Debendra Shrestha (ORCID) · **Krista Jacobsen** · **Wei Ren** · **Ole Wendroth**

Abstract Vegetable production systems are typically tillage- and input-intensive, though they may vary widely in production practices utilized. Improved understanding of soil water and nitrogen (N) processes with the use of agroecosystem models may aid in the optimization of crop yields and reduction of N losses. The objectives of this study were to (1) apply the RZ-SHAW model to diversified vegetable systems of varying production intensity, and (2) to elucidate soil N processes key loss pathways to inform opportunities for improving N cycling and sustainable intensification in these systems. The systems included conventional (CONV), low input organic (LI), and organic high tunnel (HT) vegetable systems. Soil water content and temperature were simulated well (rRMSE < 0.30) in all systems. Simulated soil NO_3^--N content was closer to measured values in the CONV than other systems. On average, the soil NO_3^--N content was underpredicted by 8 kg N ha^{-1} in the 0–0.15 m, and 5 kg N ha^{-1} in the 0.30–0.50 m soil layer in the LI system. In all systems, simulated daily N_2O flux followed the trends in the measured values, but model predicted greater peaks than measured. Nitrate leaching was the greatest N loss pathway in all systems, though timing and driving factors varied by system. Asynchrony between N mineralization and crop uptake was observed throughout the LI rotation, indicating opportunities for targeted N and irrigation inputs to increase crop yields. Simulation results indicate the need for additional study of soil microbial and N processes in HT systems.

Keywords RZ-SHAW · N_2O · High tunnels · Compost · Cropping systems · Organic agriculture

D. Shrestha (✉) · K. Jacobsen
Department of Horticulture, University of Kentucky, Lexington, KY, USA
e-mail: dshrestha5@wisc.edu

K. Jacobsen
e-mail: krista.jacobsen@uky.edu

Present Address:
D. Shrestha
Department of Agronomy, University of Wisconsin-Madison, Madison, WI, USA

W. Ren · O. Wendroth
Department of Plant and Soil Sciences, University of Kentucky, Lexington, KY, USA
e-mail: wei.ren@uky.edu

O. Wendroth
e-mail: owendroth@uky.edu

Introduction

On the global scale, vegetable production area has increased consistently at a rate of ∼ 2.5% per year

since 1980 (FAO 2018), occupying 1.1% of the world's total agricultural land in 2010 (FAO 2013). In the US, vegetable production area in 2019 amounted to 2.4 million hectares and is heavily consolidated in specialty crop-producing regions, with 76% of production occurring in California, Arizona, and Florida (USDA NASS 2020). Although covering a smaller total production area relative to staple grain crops, vegetable production systems are often input-intensive, including high nitrogen-based fertilizer applications (Rosenstock and Tomich 2016) and the use of irrigation. Linkages between inputs, cultivation practices, and environmental impacts are well documented in agronomic systems, such as the contribution of nitrogen (N) fertilizer application to air and water pollution and global climate change (Galloway et al. 2004; Tilman et al. 2011). Although vegetable production area is expanding, the body of literature on the effects of vegetable production on soil processes, greenhouse gas flux, and nutrient leaching is limited (Zhang et al. 2018). This is due, in part, to highly variable production practices specific to each crop and variety, variability in input and management intensity (Rezaei Rashti et al. 2015), and diverse rotations which may include multiple crops in a single year in many regions of the world. However, given the expanding land base and increasing intensity of vegetable and other specialty crop production systems, additional research is warranted. Further, understanding the ways in which soil organic matter and N processes vary in different vegetable farming systems provides insights for improving the overall productivity and sustainability of each production system, and vegetable-producing farms as a whole.

Although vegetable production systems have been characterized to a lesser extent compared to agronomic (e.g. grain) cropping systems, increased N losses from vegetable systems have been reported relative to other cropping systems. These include greater nitrous oxide (N_2O) fluxes and nitrate (NO_3^-) leaching losses are due, in part, to higher N fertilizer application rates compared to agronomic crop production (Liptzin and Dahlgren 2016; Xu et al. 2016). In addition to high N input requirements, vegetable production systems are commonly managed using practices known to increase N losses and greenhouse gas emissions. For example, vegetable crops are routinely grown with the scheduled application of fertilizer and irrigation (UK Cooperative Extension Service 2014), rather than precision application. Extensive soil disturbance, including raised beds and specialized mechanical cultivation, are common practices in vegetable crop production. Furthermore, the use of plastic mulch and drip irrigation, which reduce evaporation from soil and increase the water use efficiency, have been increasingly adopted in vegetable crop production globally (Lamont 1993; Darwish et al. 2003). Protected agricultural systems are growing globally as well. For example, high tunnels and other passively heated, semi-controlled structures are growing rapidly in the US, and are widely adopted in specialty crop producing regions around the world (Lamont 2009). These structures protect the crop from rainfall and typically have higher temperatures than the open field, which allows for the extension of the growing season of warm-season crops and production throughout the winter season in many temperate climates (Lamont 2009).

The intensive nature of vegetable production systems, as well as management and rotation variability, lead to more complexities in studying vegetable agroecosystems. A modeling approach may inform improved management decisions to decrease N losses, such as irrigation scheduling based on crop demand, drip irrigation, fertigation for improving synchrony between N availability and crop N demand, reduce nitrate leaching and N_2O emissions (Sun et al. 2012; Kennedy et al. 2013). Further, agroecosystem models allow a holistic perspective on nutrient management, which considers the nutrient contributions from cover crops, preceding crop and crop residues, as well as applied fertilizer inputs, which has been shown to reduce NO_3^- leaching and N_2O emissions (Crews and Peoples 2005). In addition to informing management practices, a modeling approach may be especially useful in investigating processes with high temporal and spatial variabilities, such as N_2O fluxes (Fang et al. 2015).

Process based agroecosystem models have been widely used to simulate soil water, N and carbon (C) dynamics (Ma et al. 2012), and to predict N_2O fluxes (Fang et al. 2015) and crop production (Jiang et al. 2019; Uzoma et al. 2015). RZ-SHAW is a hybrid model combining Root Zone Water Quality Model 2 (RZWQM2, Ahuja et al. 2000) and the Simultaneous Heat and Water (SHAW, Flerchinger and Saxton, 1989) model. RZWQM2 has been extensively applied

to understand soil water, N and C dynamics, N leaching, and biomass development in agronomic crops production systems such as corn, wheat, and soybean (Ma et al. 2007; Malone et al. 2007; Yu et al. 2006). However, RZWQM2 has been seldom used in vegetable production systems and diverse crop rotations, save a notable exception by Cameira et al. (2014), who used the model to study water and N budgets for organically and conventionally managed urban vegetable gardens. Recently, the RZ-SHAW model has been improved to simulate soil temperature, soil water and energy balance under plastic mulch, a practice common in vegetable production systems. To date, RZ-SHAW has been demonstrated to effectively simulate crop growth and soil N processes, e.g. NO_3^- leaching (Kozak et al. 2006; Gillette et al. 2017; Jiang et al. 2020) and crop yield. However, RZ-SHAW has not been utilized to simulate soil water, soil mineral N dynamics, N_2O flux, or crop yields under plastic mulch conditions, save the notable exception of Zhou et al. (2020), who used the RZ-SHAW model to evaluate soil temperature under plastic mulch conditions. The objectives of this study were to (1) apply the RZ-SHAW model to diversified vegetable systems of varying production intensity, and (2) to elucidate soil N processes key loss pathways to inform opportunities for improving N cycling and sustainable intensification in these systems.

Materials and methods

Field experiment and data collection

This study was initiated in early spring 2014 at two sites in central Kentucky with Maury silt loam soil (a fine, mixed, active, mesic Typic Paleudalf); the University of Kentucky Horticulture Research Farm (UK HRF) in Lexington, KY (37°58′29″N, 84°32′05″W), and a local farm in Scott County, Kentucky (38°13′20″N, 84°30′38″W). Both farms share similar soil and climatic conditions. The annual rainfall was 1209, 1475, and 1011 mm, and the average air temperature was 12 °C, 13.3 °C and 14.2 °C in 2014, 2015, and 2016, respectively. Each system contained six replicate plots.

Three vegetable production systems representing varying levels of agricultural intensification were utilized, as characterized by the nature and length of

fallow periods, tillage intensity, irrigation, and nutrient inputs. The three study systems included (1) a Low Input Organic (LI) system on the local farm, (2) a Conventional (CONV) diversified vegetable production system at the UK HRF, managed according to standard commercial vegetable production recommendations in the region (UK Cooperative Extension Service 2014), and (3) an Organic High Tunnel (HT) system on the UK HRF, an intensive system managed for diversified, year-round vegetable crop production. Key management dates, input rates and timing, and a description of nutrient and water management practices are described below. Additional management details for each system can be found in Shrestha et al. (2019).

The CONV system consisted of a winter wheat (*Triticum aestivum* L.) cover crop during winter, followed by a spring vegetable crop in the years when a cool season crop was not planted. Fertilizers were applied according to split-application recommendations for each crop (UK Cooperative Extension Service 2014). Fertilizers applied prior to planting were balanced mineral fertilizers (Miller 19–19-19, Miller Chemical and Fertilizer, Hanover, PA) at the rate of 78 kg N ha^{-1} for peppers, and 56 kg N ha^{-1} for beets, collards, and beans. Peppers and collards received supplemental in-season fertigation with calcium nitrate fertilizer (13–0-0, PureCal, Master Plant-Prod Inc., Brampton, ON) at a rate of 9 kg N ha^{-1} per application at five different application dates. In the CONV system, peppers were transplanted on May 20, 2014, beets were seeded on April 24, 2015, collards were transplanted on August 19, 2015, and beans were seeded on May 7, 2016.

The Low Input Organic system (LI) consisted of a five-year mixed grass/legume pasture followed by a three-year rotation of annual vegetable crops. The LI system did not receive any supplemental fertilizer. Crops in the LI system were exclusively dependent on natural rainfall except for peppers, which received drip irrigation at the start of the growing season. In the LI system, peppers were transplanted on May 14, 2014, beets were seeded on June 8, 2015, collards were transplanted on October 11, 2015, and beans were seeded on May 28, 2016.

The Organic High Tunnel system (HT) consisted of three replicated 9.1 m × 22 m unheated greenhouse structures. Temperature and ventilation were controlled by manual manipulation of doors and plastic

curtains. Pre-plant fertilizer consisted of composted horse manure compost applied at a rate of 24-ton ha^{-1} and a granular organic fertilizer (Harmony 5–4-3, BioSystems, LLC, Blacksburg, VA) applied at a rate of 67 kg N ha^{-1} before each crop. In addition to pre-plant fertilizer, peppers were fertigated in-season with liquid organic fertilizer (Brown's Fish Fertilizer 2–3-1, C.R. Brown Enterprises, NC) at the rate of 28 kg N ha^{-1} per application, applied twice during the growing season. All crops were drip irrigated using municipal water, as the structures exclude rainfall. Crops were irrigated every two to three days in summer and every three to four days in winter, depending on soil moisture status. Irrigation lasted for two to four hours and occurred at a rate of 0.0066 m hr$^{-1.}$ In the HT system, peppers were transplanted on April 22, 2014, beets were seeded on March 12, 2015, collards were transplanted on September 25, 2015, and beans were seeded on April 28, 2016.

Soils were sampled monthly at 0–0.15, 0.15–0.30, and 0.30–0.50 m depths for NO_3^--N from six replicate plots. Soil NO_3^--N was extracted from a 5 g subsample of fresh soil in 1 M KCl (Rice and Smith 1984) and analyzed via microplate spectrophotometer (Epoch Model, BioTek Instruments, Inc., Winooski, VT, USA). N_2O flux was measured bi-weekly using an FTIR-based field gas analyzer (Gasmet DX4040, Gasmet Technologies Oy, Helsinki, Finland). Rectangular stainless-steel chambers (0.164 m × 0.527 m × 0.152 m) were installed in each plot. Gas fluxes were calculated using the following equation by Iqbal et al. (2013):

$$F = \frac{\Delta C}{\Delta t} \frac{V}{A} \rho \qquad (1)$$

where F is the gas flux rate (mg m^{-2} h^{-1}), $\Delta C/\Delta t$ denotes the increase/decrease of gas concentration (C) in the chamber over time (t), V is the chamber volume (m^3), A is the chamber cross-sectional surface area (m^2), denotes the gas density at 25 °C. Cumulative gas fluxes were calculated by interpolating trapezoidal integration of flux versus time between sampling dates and integrating the area under the curve (Venterea et al. 2011).

Soil water potential at three depths in the soil profile (0.10, 0.30, and 0.50 m) and soil temperature at 0.10 m depth were measured using granular matrix sensors (Watermark, Irrometer Co., Riverside, CA).

Soil temperatures were measured at the time of N_2O flux measurement with a digital soil thermometer inserted at 0.10 m soil depth.

Plant biomass samples were dried at 60 °C until a constant mass was achieved, homogenized on a Wiley Mill (Thomas Scientific, Swedesboro, NJ), and a subsample ground on a roller mill (Model 764AVM, U.S. Stoneware, East Palestine, OH). The entire plant biomass of one plant from each plot for each crop was analyzed for percent C and N on an elemental analyzer (Thermo Scientific FlashSmart, CE Elantech, Lakewood, NJ).

Model description

Root Zone Water Quality Model 2 (RZWQM2) is a one-dimensional agricultural system model, which simulates mineralization and immobilization of crop residues, mineralization of soil N, volatilization, nitrification, and denitrification (Ahuja et al. 2000). The model also simulates soil water content, nutrient leaching, and crop yield. The agricultural management options in RZWQM2 include crop and crop cultivar selection, planting date, manure, fertilizer and pesticide application, tillage, and irrigation (Ma et al. 2012). Brooks–Corey equations are used to relate volumetric soil water content (θ), hydraulic conductivity (K), and soil suction head (h) (Ma et al. 2012). The N_2O emission algorithm in RZWQM2, as described in Fang et al. (2015), was adapted from the DAYCENT model (Parton et al. 1998; Del Grosso et al. 2000) and Nitrous Oxide Emission (NOE) model (Hénault et al. 2005). The RZ-SHAW model utilizes the major features of the RZWQM2 described above, where the RZWQM2 sub model provides soil water content, root distribution, soil evaporation, soil transpiration, leaf area index, and plant height at each time step to the SHAW sub model. In turn, SHAW supplies soil ice content, updated soil water content due to ice and freezing, and soil temperature to RZWQM2 (Fang et al., 2014). Modifications to simulate the effect of plastic mulch on soil temperature has been included in RZ-SHAW version 4.0, which assumes that soil water is evaporated only from non-mulched areas and ignores the head transfer by evaporation and condensation between the mulch and the soil surface (Zhou et al. 2020). Additional details about the RZ-SHAW model can be found in Gillete et al. (2017).

Model input, calibration, and validation

For the CONV and LI systems, weather input data, including daily minimum and maximum air temperatures, wind speed and direction, shortwave radiation, and relative humidity, were obtained from the Kentucky Mesonet (KYMESONET 2018). Daily precipitation data for the LI systems were taken from a regional airport located approximately 8 km distance from the research site (NOAA 2018).

Plastic mulches were used in the pepper and collard crops in the CONV system and for the pepper crop in the LI system. Plastic mulches covered planting beds that were raised approximately 0.15 m high and 0.50 m wide, with approximately 1 m between the center of each bed. The furrow between the raised beds was left uncovered. Circular holes of approximately 0.06 m in diameter were punched through the plastic cover for planting peppers and collards in the CONV system and peppers in the LI system. For the HT system, daily maximum, minimum temperature, and relative humidity values were summarized from data loggers measuring at 15-min intervals, mounted 2 m high in the center of the structures (WatchDog B102, Spectrum Technologies, Aurora, IL). The daily solar radiation inside tunnels was calculated as the product of solar radiation outside and tunnel plastic roof transmissivity, as described in VegSyst V2 model (Gallardo et al. 2016):

$$SR_{in} = SR_{out} \times \tau \quad (2)$$

where SR_{in} denotes the incoming solar radiation, SR_{out} is the outgoing solar radiation, and τ is the transmissivity of the double-layer polyethylene sheet cover on the high tunnel equal to 0.7 according to Biernbaum (2013).

The simulation began on January 1, 2014 and ended on December 31, 2016 in all systems. The model was calibrated with the CONV system data and validated with the LI and HT systems. Soil texture data and soil water content at 1/3 and 15 bar of soil were obtained from the USDA NRCS Web soil survey (Web Soil Survey 2018) (Table 1). Saturated hydraulic conductivity, soil water content at 1/3 bar and 15 bar in the CONV system were calibrated based on the measured soil water content in the CONV system. Initial total C content at the depth of 0–0.15 m, 0.15–0.30 m, and 0.30–0.50 m were 1.10%, 1.09%, and 0.83% in CONV system; 1.75%, 1.31%, and 0.87% in LI

system; and 1.56%, 1.48%, and 1.12% in the HT system. Initial values for fast and slow residue pools, slow, medium, and fast soil humus pools, and microbial pools were calculated based on measured soil carbon data. As recommended by the model developers, a 10-year "warm-up" run was conducted under current weather and management practices for the CONV and HT system to obtain stable soil residue and microbial pools.

In the LI system, the vegetable crops were grown in the field, which was converted from pasture and had not been tilled for five years. Thus, the initial carbon pool values in the LI system were obtained from the "warm up" run without tillage operation to mimic the pasture production system (Feng et al. 2015). Model default values were used for initial soil chemical conditions. Crop parameters were calibrated with the measured yield component data from the CONV system and validated with the HT and LI systems. For the pepper crop, crop parameters were obtained from DSSAT pepper variety 'Capistrano', as plant height, leaf structure, and fruit type were similar to pepper variety 'Aristotle' grown in the study. Dry bean variety 'Andean Habit 1′ was chosen for the fresh bean crop in the rotation, as its plant characteristics were close to the variety 'Provider' grown in our experiments. For the table beet plant parameters, the DSSAT sugar beet variety 'SVRR1142E' was selected. Sugar beet crop parameters that were modified to more closely replicate a table beet variety include G2 leaf expansion rate during stage 3 to 130 m^2 m^{-2} day^{-1}, G3 root tuber growth rate to 0.0145 kg m^{-2} day^{-1} and plant biomass at half of the maximum height to 0.00907 kg $plant^{-1}$ (Tei et al. 1996). The cabbage variety '990,001 Tastie 4′ parameters were modified to simulate the collard crop. The specific leaf area of this cultivar under standard growth conditions (SLAVR) was modified to 8 m^2 kg^{-1} (Uzun and Kar 2004) and for the maximum size of the full leaf (three leaves) (SIZLF) the measured value of 0.035 m^2 was entered. The DSSAT cabbage crop parameters were modified to mimic the lettuce crop used in our study; SLAVR was modified to 10 m^2 kg^{-1} (Tei et al. 1996) and SIZLF was modified to 0.025 m^2. The model performance in simulating the soil temperature, soil water, soil NO_3^--N, and N_2O flux was evaluated with the coefficient of determination (R^2), root mean square error (RMSE), and mean difference (MD) as described

Table 1 Soil bulk density, soil textural and calibrated hydraulic properties used for RZ-SHAW simulation

Soil depth (m)	Bulk density (kg m^{-3})	Soil texture			Saturated hydraulic conductivity K_{sat} mm hr^{-1}	Soil water content			
		Sand	Silt %	Clay		$\theta_{1/3}$ (m^3 m^{-3})	θ_{15}	$\mathbf{\theta_s}$	θ_r
0–0.15	1330	7	76	17	6.8	0.29	0.13	0.54	0.01
0.15–0.30	1380	7	76	17	6.8	0.29	0.14	0.49	0.01
0.30–0.50	1410	6	65	29	1.5	0.31	0.19	0.46	0.04
0.50–0.70	1450	6	65	29	1.5	0.31	0.21	0.45	0.04
0.70–1.00	1470	6	62	32	1.5	0.32	0.22	0.44	0.04

Soil texture, saturation (θ_s), 1/3 bar ($\theta_{1/3}$), 15 bar (θ_{15}) and residual (θ_r) soil water content values for model calibration were taken from USDA NRCS Web Soil Survey (Soil Survey Staff 2018)

in Gillette et al. (2017); and Relative RMSE (rRMSE) as described in Anar et al. (2020).

$$R^2 = \left(\frac{\sum_{i=1}^{N}(O_i - O_a)(P_i - P_a)}{\sqrt{\sum_{i=1}^{N}(O_i - O_a)^2 \sum_{i=1}^{N}(P_i - P_a)^2}} \right)^2 \quad (3)$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2} \quad (4)$$

$$MD = \frac{\sum_{i=1}^{N}(P_i - O_i)}{N} \quad (5)$$

$$nRMSE = \frac{RMSE}{Oa} \quad (6)$$

Results

Soil temperature and water dynamics

RZ-SHAW simulated soil temperature at the 0.10 m depth reasonably well in the three systems, with rRMSE values of 0.35 for the CONV, 0.29 for the LI,

and 0.18 for the HT (Table 2). RZ-SHAW underestimated soil temperature by 3.31 °C in the CONV system and 3.86 °C in the LI system but was nearly equal to field measurements in the HT system when averaged across the three-year rotation (Table 2).

The simulated and measured soil water content at three different soil depths (0.10 m, 0.30 m, and 0.50 m) in the CONV, LI, and HT systems at all depths are presented in Table 3 and Figs. 1, 2, and 3. On average, measured soil water content in the CONV system was close to the simulated values at 0.10 m and 0.30 m, but was underpredicted by 6% at 0.50 m (Table 3). RZ-SHAW underestimated soil water content during high soil moisture conditions but overestimated during drier soil conditions. In the CONV system, there was poor agreement between measured and simulated soil water content at three soil layers with R^2 value less than 0.26. The greatest underestimations of soil water content at the 0.50 m soil depth occurred during the pepper and collard crops in the CONV system (Fig. 1), which were grown in a raised bed covered by plastic mulch.

In the LI system, soil water content values were overpredicted by 16% at 0.10 m, 20% at 0.30 m, and

Table 2 Soil temperature as measured in the field and simulated by RZ-SHAW at the 0.10 m depth and R^2, root mean square error (RMSE), relative root mean square error (RRMSE), and mean difference (MD) for the conventional (CONV), low input organic (LI), and organic high tunnel (HT) production systems

System	Measured (°C)	Simulated (°C)	R^2	RMSE (°C)	rRMSE	MD (°C)
CONV	12.3	10.4	0.90	4.33	0.35	− 3.31
LI	17.6	15.7	0.83	5.10	0.29	− 3.86
HT	16.6	16.6	0.87	3.03	0.18	− 0.62

Table 3 Measured and simulated soil water content, averaged over three-year period, at three different depths (0.10, 0.30, and 0.50 m) in conventional (CONV), low input organic (LI), and organic high tunnel (HT) production systems

System	Soil depth (m)	Measured average m^{-3} m^{-3}	Simulated average m^{-3} m^{-3}	R^2	RMSE m^{-3} m^{-3}	rRMSE	MD m^{-3} m^{-3}
CONV	0.10	0.36	0.36	0.26	0.06	0.17	0.00
	0.15–0.30	0.38	0.39	0.14	0.06	0.17	0.01
	0.30–0.50	0.42	0.39	0.02	0.05	0.12	− 0.02
LI	0–0.15	0.29	0.34	0.48	0.07	0.26	0.05
	0.15–0.30	0.31	0.37	0.66	0.08	0.25	0.06
	0.30–0.50	0.34	0.37	0.65	0.07	0.20	0.03
HT	0–0.15	0.26	0.30	0.46	0.07	0.28	0.04
	0.15–0.30	0.31	0.33	0.43	0.07	0.22	0.02
	0.30–0.50	0.34	0.34	0.29	0.07	0.20	0.00
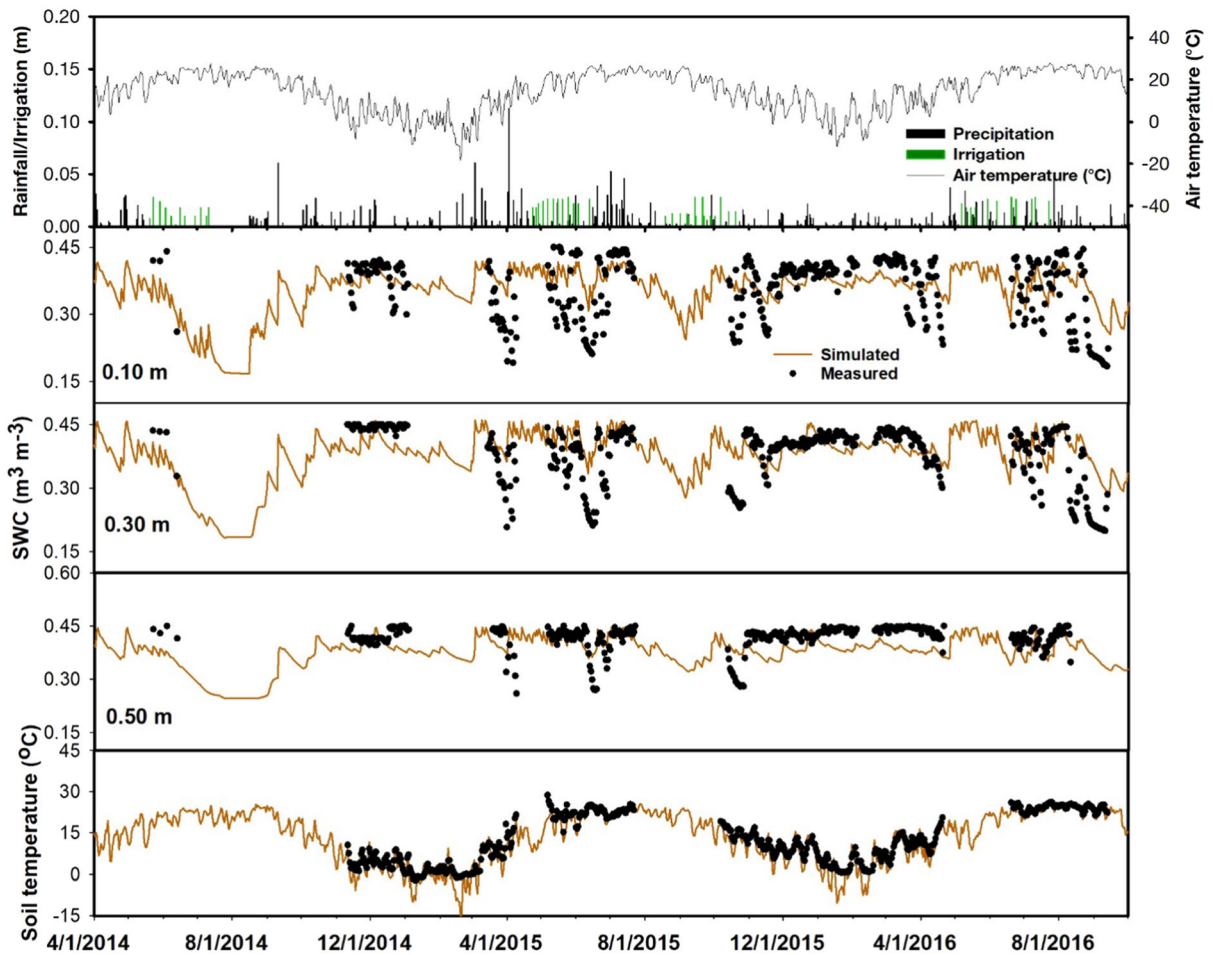
Fig. 1 Measured and RZ-SHAW simulated soil water content measured at 0.10 m, 0.30 m, and 0.50 m, and soil temperature measured at 0.10 m in conventional System (CONV) over the simulation period of 2014–2016
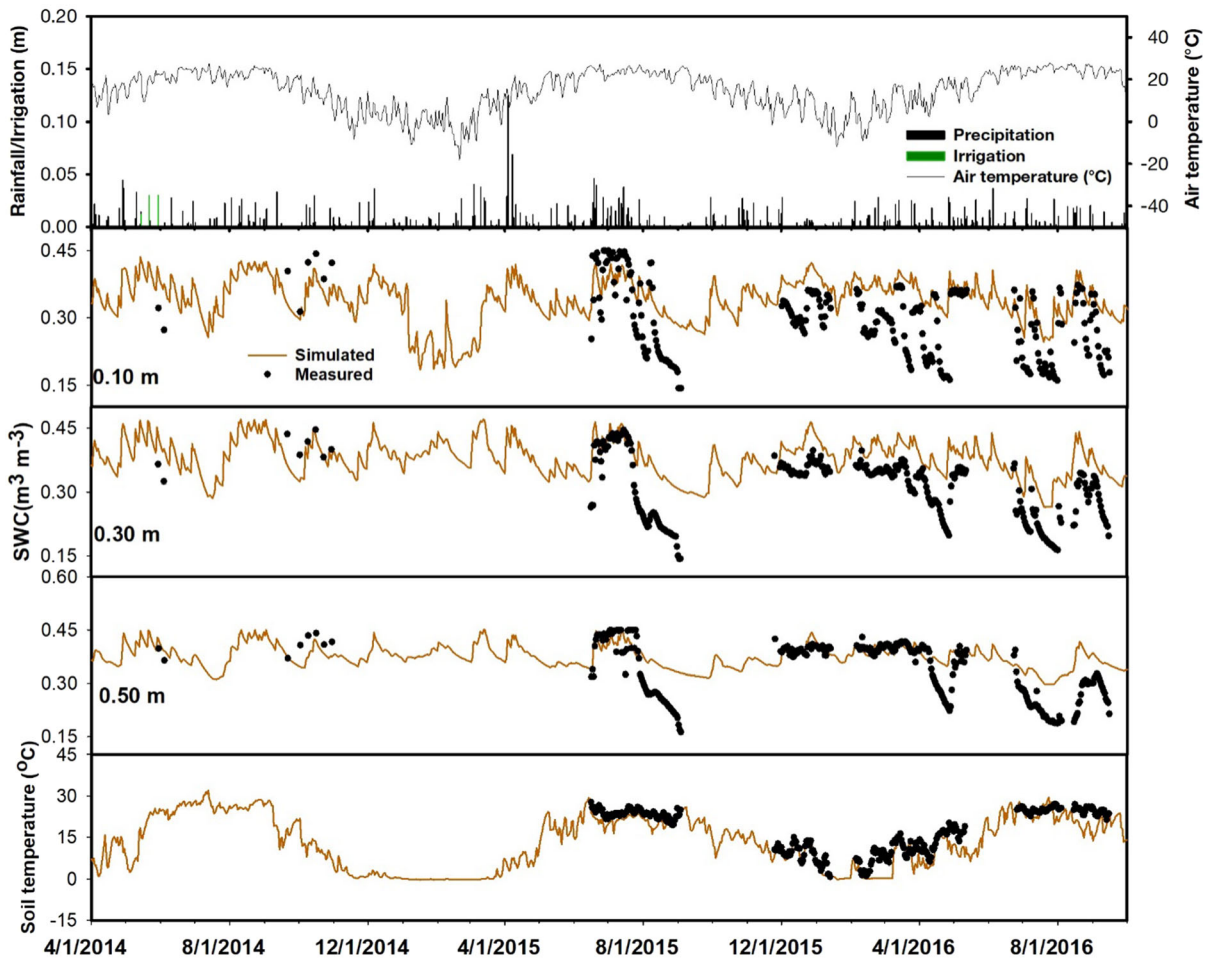
Fig. 2 Measured and RZ-SHAW simulated soil water content measured at 0.10 m, 0.30 m, and 0.50 m, and soil temperature measured at 0.10 m in low input organic system (LI) over the simulation period of 2014–2016

10% at 0.50 m soil depth on average (Table 3). Model fit statistics demonstrate better agreement between simulated and measured values at the 0.30 m depth, followed by 0.50 and 0.10 m soil depths, as indicated by higher R^2 and lower RMSE values (Table 3, Fig. 2).

Soil water content values in the HT system was overpredicted by 13% at 0.10 m and 5% at 0.30 m, while average measured soil water content was equal to simulated values at 0.50 m soil depth. R^2 values greater than 0.43 at 0.10 m and 0.30 m soil depth showed better agreement between simulated and observed soil water content than 0.50 m soil depth. The observed soil water content values at 0.10 m depth were fluctuated largely than the simulated values.

Soil nitrate dynamics

The efficiency of RZ-SHAW to simulate NO_3^--N dynamics as shown by R^2 and RMSE values differed with varied soil and crop management practices and environmental conditions inherent to CONV, LI, and HT systems (Table 4, Fig. 4a-c). RZ-SHAW underestimated soil NO_3^--N content in all systems and in all three soil layers. The difference between the simulated and measured soil NO_3^--N content was comparatively greater in 0–0.15 m and 0.30–0.50 m soil layer compared to 0.15–0.30 m soil layer during both model calibration and validation (Table 4). Within the individual soil layers, the model agreement was reasonable at all three soil layers, with R^2 and RMSE values of 0.32 and, RMSE = 38 kg N ha^{-1} in the
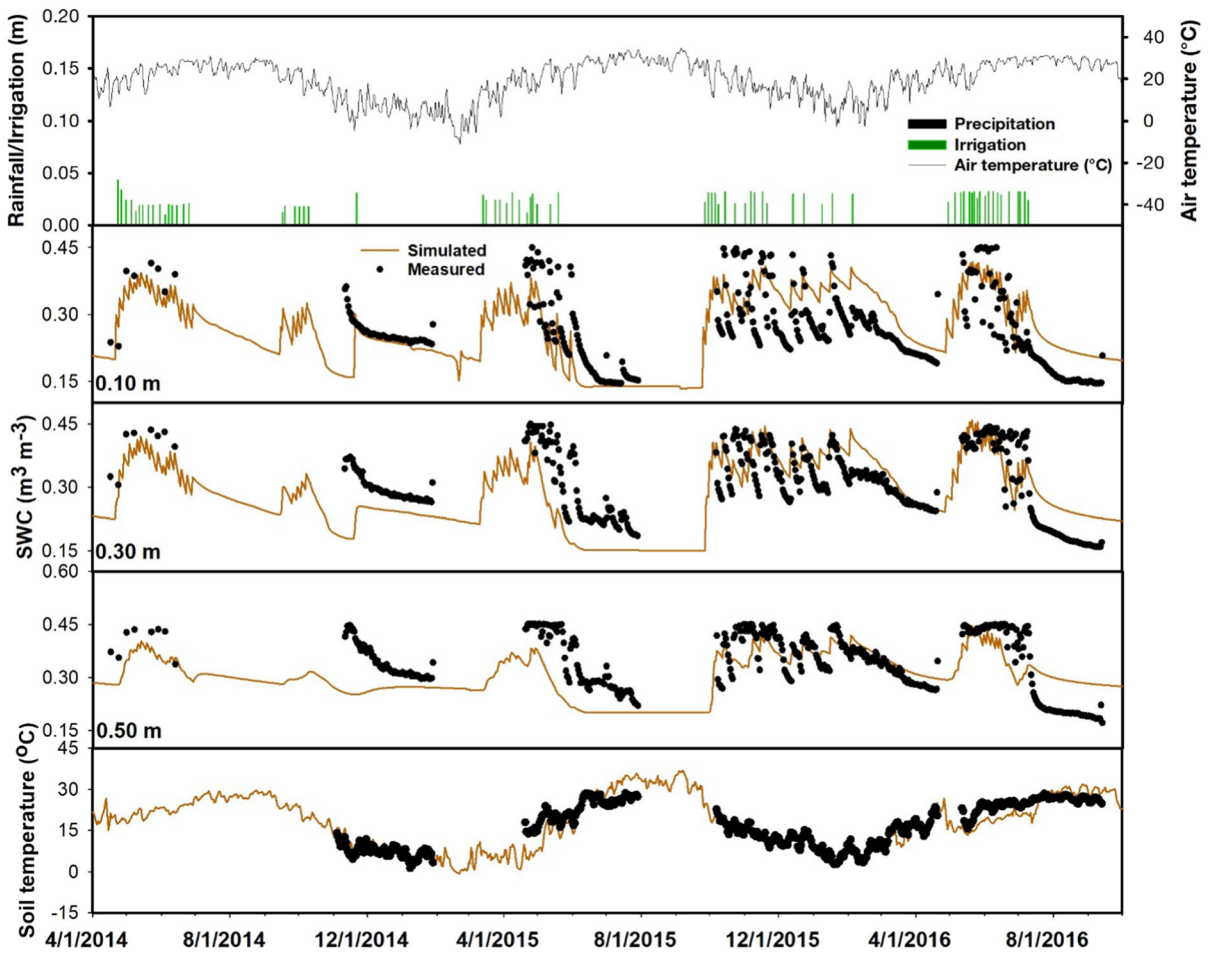
Fig. 3 Measured and RZ-SHAW simulated soil water content at 0.10 m, 0.30 m, and 0.50 m, and soil temperature at 0.10 m in high tunnel organic system (HT) over the simulation period of 2014–2016

Table 4 Measured and simulated average soil NO_3^--N content at 0–0.15 m, 0.15–0.30 m, and 0.30–0.50 m soil layers in conventional (CONV), low input organic (LI), and organic high tunnel (HT) production systems

	Soil depth m	Measured average kg N ha^{-1}	Simulated average kg N ha^{-1}	R^2	RMSE kg N ha^{-1}	rRMSE	MD kg N ha^{-1}
CONV	0–0.15	31.2	17.9	0.32	38.34	1.23	-13.29
	0.15–0.30	23.0	19.0	0.22	24.74	1.08	-3.93
	0.30–0.50	25.0	13.1	0.47	25.24	1.01	-11.86
LI	0–0.15	18.6	10.5	0.10	19.04	1.02	-8.14
	0.15–0.30	10.8	10.1	0.59	6.55	0.60	-0.69
	0.30–0.50	13.3	8.2	0.18	11.23	0.85	-5.09
HT	0–0.15	64.2	38.9	0.09	82.40	1.28	-27.64
	0.15–0.30	20.9	14.1	0.02	18.95	0.91	-6.83
	0.30–0.50	41.8	8.9	0.01	51.08	1.22	-32.85
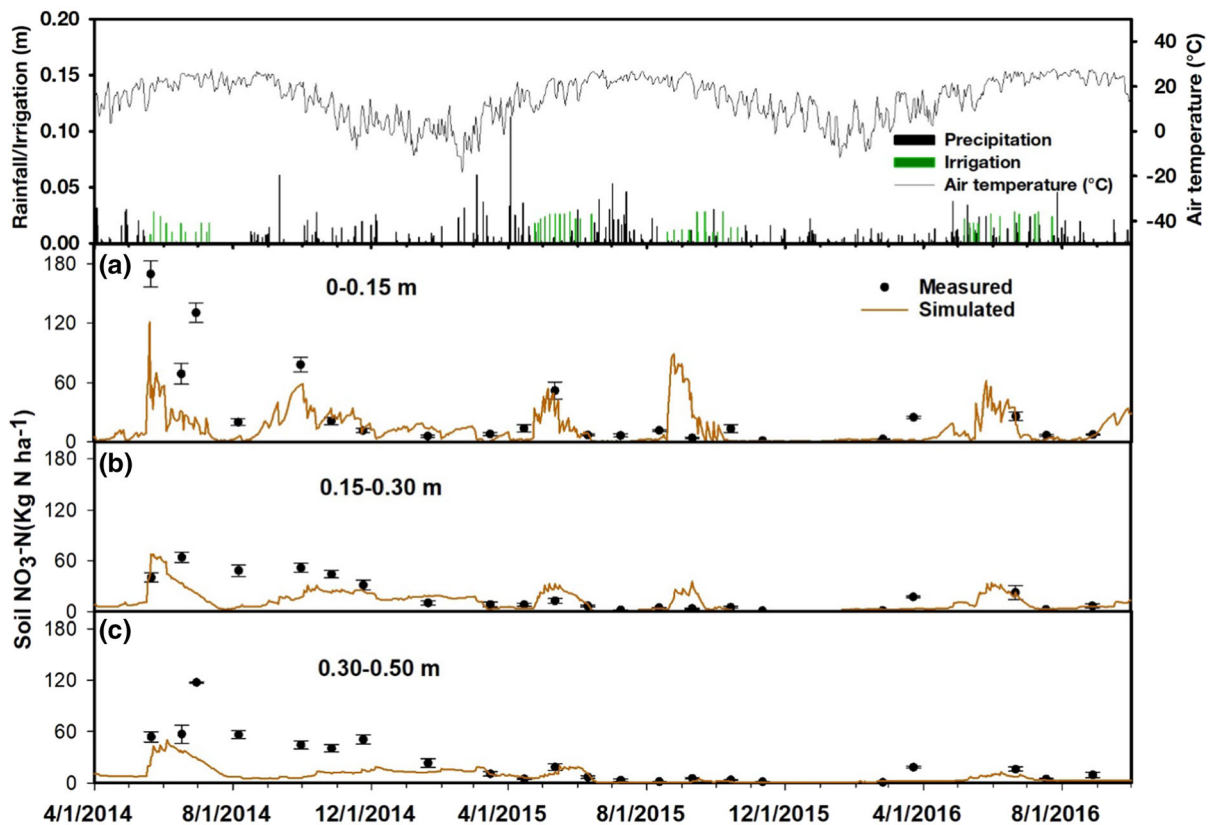
Fig. 4 Measured and simulated soil NO$_3^-$-N in **a** 0–0.15 m **b** 0.15–0.30 m, and **c** 0.30–0.50 m soil layer in the conventional System (CONV) over the simulation period of 2014–2016

0–0.15 m, 0.22 and 25 kg N ha^{-1}, and 0.47 and 25 kg N ha^{-1} in the 0.50 m soil layer (Table 4). Averaged over the entire simulation period, soil NO$_3^-$-N was under-predicted with mean difference of 13 kg N ha^{-1} in the 0–0.15 m, 4 kg N ha^{-1} in the 0.15–0.30 m, and 12 kg N ha^{-1} in the 0.30–0.50 m soil layer.

In the LI system, RZ-SHAW under-predicted the soil NO$_3^-$-N content by 8 kg N ha^{-1} in the 0–0.15 m layer and 5 kg N ha^{-1} in the 0.30–0.50 m layer, while it over-predicted the NO$_3^-$-N in the 0.15–0.30 m soil layer by 1 kg N ha^{-1} (Table 4). Overall model agreement was considerably lower in the 0–0.15 m soil layer in the LI system, partially due to differences between simulated and measured values on several sampling dates (Fig. 5a). In the 0–0.15 m layer, R^2 values increased from 0.10 to 0.44 and RMSE value reduced from 19 to 11 kg N ha^{-1} if the August 7, 2014 and April 15, 2015 dates were not included. However, measured values from these dates were

included in the values reported here, as they were not clear outliers in the data set. The poor agreement between measured and simulated values for these sampling dates might be related to the disturbance of the surface soil before soil sampling dates by the uprooting of pepper plants after harvesting in 2014 and tillage before planting of beets in 2015. There was poor agreement between measured and simulated NO$_3^-$-N in the HT system in all three soil layers, as shown by low R^2 and high RMSE values (Table 4). This discrepancy was greater in 0–0.15 m and 0.30–0.50 m soil layers (Fig. 6).

Nitrous oxide flux in vegetable systems

Measured and simulated daily N$_2$O flux in the CONV, LI, and HT system are presented in Figs. 7a–c. In all systems, simulated daily N$_2$O flux followed the trends in the measured values, but in general, the simulation predicted a more dynamic flux pattern and greater
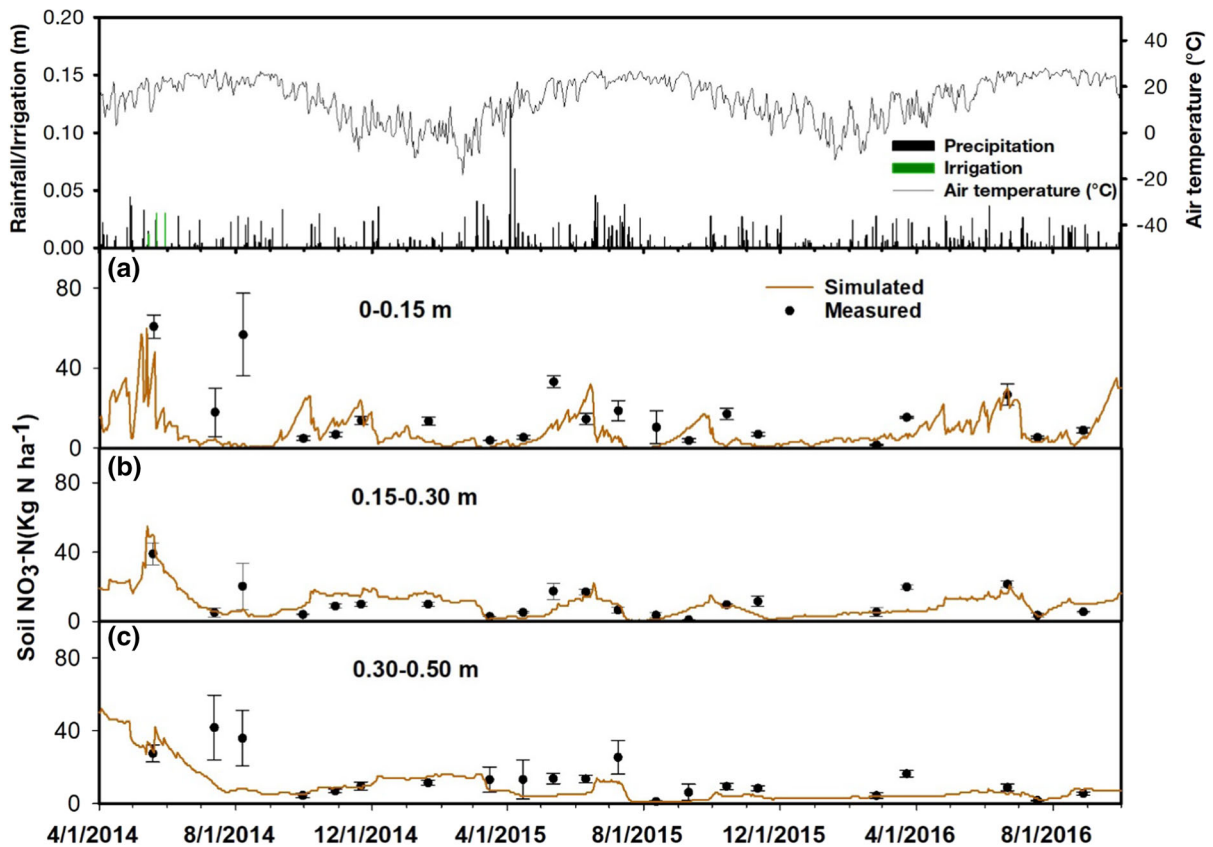
Fig. 5 Measured and simulated soil NO_3^--N in **a** 0–0.15 m **b** 0.15–0.30 m, and **c** 0.30–0.50 m soil layer in low input system (LI) over the simulation period of 2014–2016

peak values than captured by the bi-weekly gas flux measurements. R^2 and RMSE values for daily N_2O flux ranged from 0.06 to 0.67 and 7 to 38 g N_2O-N ha^{-1} day^{-1}.

In the CONV system, the cumulative N_2O-N flux was overpredicted by 4.8 kg N_2O-N ha^{-1} (Table 5). The large mismatch between the simulated and observed N_2O flux values in the CONV system was observed at the start of the pepper growing season, which accounted for over half (90%) of cumulative 170% overprediction of N_2O-N flux for the entire rotation (Fig. 7a).

Daily N_2O flux was well predicted in the HT system, with RMSE value 7.4 g N_2O-N ha^{-1} day^{-1} (Table 5). The simulated cumulative N_2O flux value was underpredicted by 16% in the HT system (Table 5). In the LI system, the cumulative N_2O-N flux over the three-year simulation period was underpredicted by 2.1 kg N_2O-N ha^{-1}, which may be

related to the underestimation of soil NO_3^--N content in the 0–0.50 m soil profile (Table 5).

Crop yields and biomass N

Crop yield and biomass N were simulated using existing crop growth modules in RZ-SHAW that had similar morphological characteristics and yield potentials of the vegetable varieties used in this study. In general, crop biomass and yield were simulated well in all crops and systems except the beets grown in the HT system (Table 6). This is of note, particularly because simulated values in several crops that use soil management practices that affect soil water content and crop nutrient uptake, such as plastic mulches and raised beds, are novel to RZWQM2. Moreover, weed biomass, which was significant in the LI system, was not included in the simulations. Simulated crop yields for all crops were overestimated in the CONV and LI systems, while underestimated in the HT system,
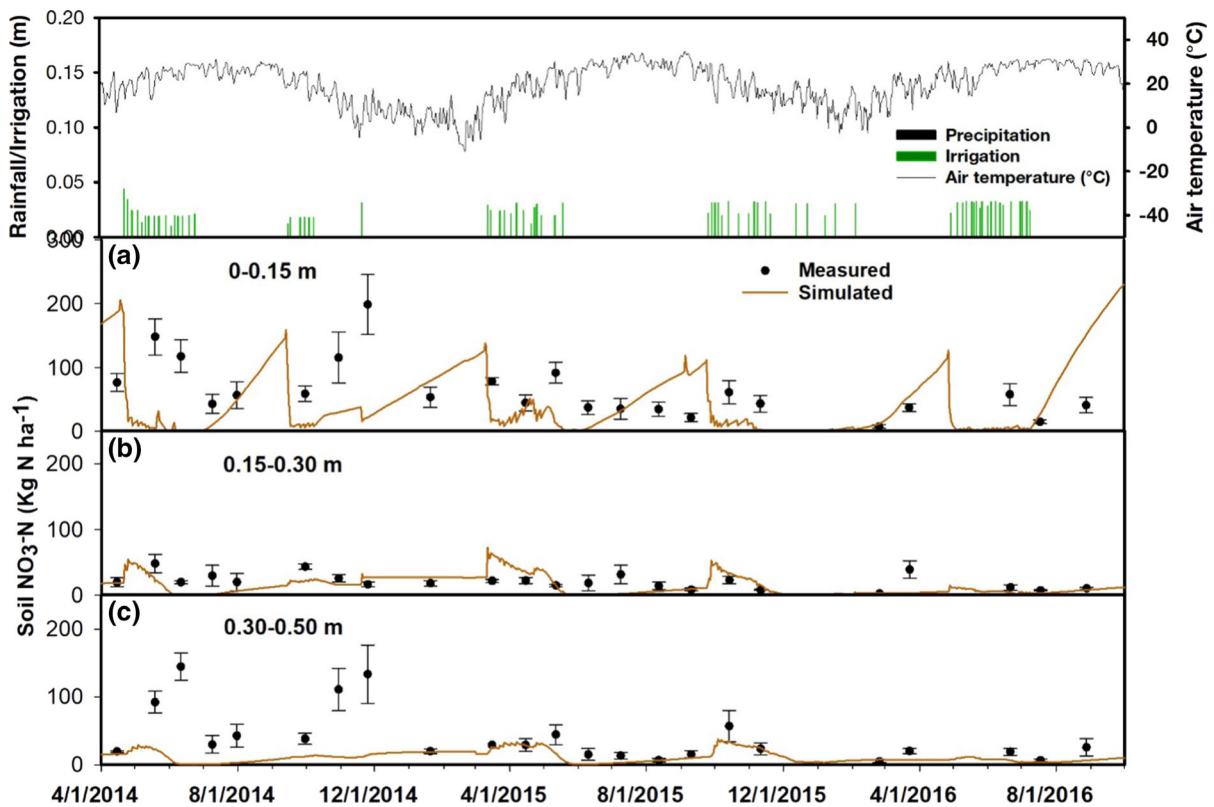
Fig. 6 Measured and simulated soil NO$_3^-$-N in **a** 0–0.15 m **b** 0.15–0.30 m, and **c** 0.30–0.50 m soil layer in the high tunnel organic system (HT) over the simulation period of 2014–2016
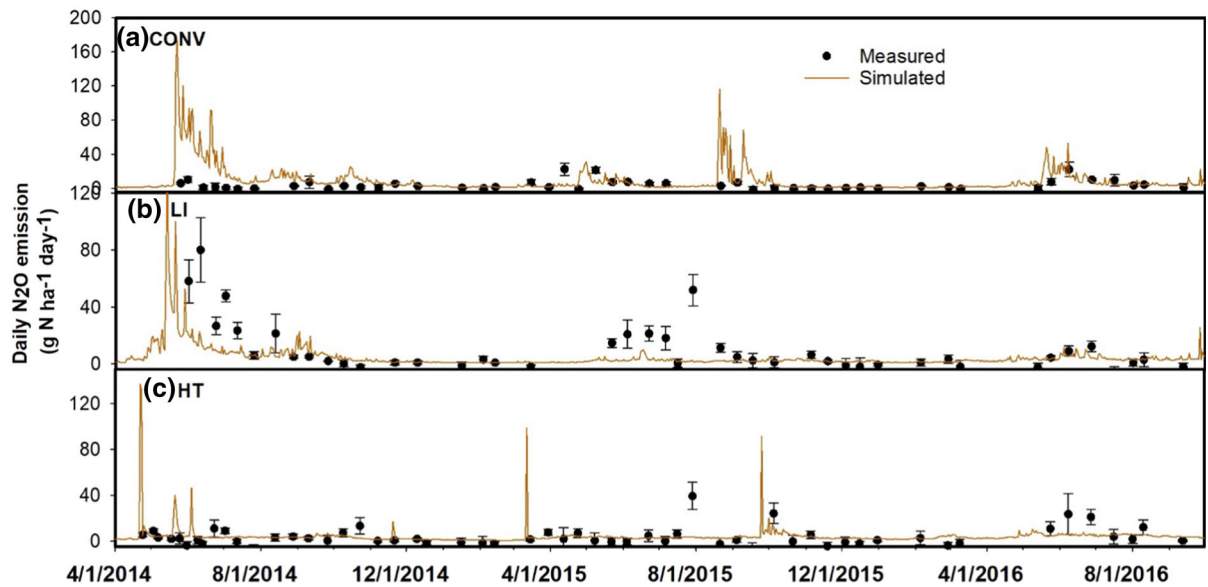
Fig. 7 Measured and RZ-SHAW simulated daily N$_2$O emission in in conventional (CONV), low input organic (LI), and organic high tunnel (HT) production systems over the simulation period of 2014–2016

Table 5 Measured and simulated cumulative soil N_2O-N flux over the simulation period of three years from 2014 to 2016

	Measured total kg N_2O-N ha^{-1}	Simulated total kg N_2O-N ha^{-1}	R^2	RMSE g N_2O-N ha^{-1}	MD g N_2O-N ha^{-1}
CONV	2.8	7.6	0.1	38.1	14.2
LI	5.7	3.6	0.7	15.9	0.1
HT	4.5	3.8	0.1	7.4	-0.3

Model fit statistics: R^2, RMSE, and MD values were analyzed with daily soil N_2O-N flux (kg N_2O-N ha^{-1})

Table 6 Measured and simulated biomass N and crop yield (Dry matter basis) of pepper, beets, collards, and beans in conventional (CONV), low input organic (LI), and organic high tunnel (HT) production systems

		Biomass N kg N ha^{-1}		Yield kg ha^{-1}	
		Measured	Simulated	Measured	Simulated
CONV	Pepper	187	212	4128	4521
	Beets	144	124	5805	11,075
	Collards	162	144	3599	5498
	Beans	153	142	2739	3541
LI	Pepper	127	129	2669	3476
	Beets	10	67	487	7407
	Collards	15	3	469	67
	Beans	82	111	576	871
HT	Pepper	234	227	5944	4357
	Beets	121	127	4936	11,134
	Collards	167	123	3976	2354
	Beans	112	103	1220	326

except for the HT beet crop. Table beet yield and biomass were not simulated well by the model in any system.

Discussion

Soil N processes and dynamics are controlled by the interactive effect of soil temperature, and soil moisture (Guntiñas et al. 2012; Xu et al. 2016; Thies et al. 2020), the nature of inputs (Doltra et al. 2019) and degree of disturbance (Dobbie et al. 1999; Kristensen et al. 2000; Congreves et al. 2017) which varies among different agroecosystems and with different agricultural management and growing environments. Vegetable production systems are often complex with inclusion of production practices such as plastic mulch, raised bed, drip irrigation, and protected agriculture systems (Carey et al. 2009). Given the dynamic nature of soil water and N processes, it is not always possible to understand or predict their status at a given time solely with field measurements without extreme sampling rigor. Agroecosystem models may improve our understanding of these processes, although no model provides an exact simulation for field conditions. The RZ-SHAW introduced a plastic mulch option, and this effort represents the first attempt to date to utilize this option for predicting soil water, soil N, and N_2O flux in diversified vegetable systems. Model fit was poor in some portions of the rotation due, likely due to the use of uncommon production practices (e.g. pasture inversion), production conditions novel to the model (e.g. protected agriculture systems), and the use of model crop options with different morphology than the varieties utilized in this study. However, the simulation effort offers information on key N loss pathways in each of these systems, which vary by level of intensification, and identify opportunities for improving management.

RZ-SHAW model fit affected by use of novel rotation practices and plasticulture

Soil temperature and water processes

Overall model fit was acceptable for simulating soil temperature and soil water content in all systems, based on a threshold of relative root mean square error (rRMSE) values < 0.30 (Shahadha et al. 2019; Anar et al. 2020). Overestimation of soil water content was pronounced in the LI system in each soil layer with RMSE values greater than 0.07 m^3 m^{-3} and MD greater than 0.03 m^3 m^{-3}. Weed growth was likely responsible for large uptake of the soil water and reduced the amount of water from the soil, which could not be accounted for by the model simulation. Similar results were reported by Shahadha et al. (2019), who used RZWQM2 to simulate soil water content under soybean and corn grown in the same soil series and region as in this study (Maury silt loam, Kentucky, USA), who reported RMSE values ranging from 0.07 to 0.11 m^3 m^{-3} at 0.10 m soil depth and 0.05 to 0.08 m^3 m^{-3} at 0.30 m soil depth.

In the CONV system, lack of overall model fit between measured and simulated soil water values were driven by large discrepancies during the pepper and collard growing periods, which were grown on a raised bed with plastic mulch. Water was observed to accumulate in the alley between the mulched raised beds during rainfall events and percolated into the soil under the mulch bed, which may have resulted in the high measured soil water content in the deep layer. Further, soil water content was observed to be higher in the zone near the planting hole in the plastic mulch than the surrounding area during periods of high rainfall, as observed in other work (e.g. Chen et al. 2018).

Discrepancies in soil water and temperature dynamics N processes in the HT system may be attributed to the novel environment inside the high tunnel structure. As the structure excludes rainfall, the soil in the HT system was severely water limited during fallow periods (Lamont 2009) and irrigation was discontinued during fallow periods. Limited soil water during fallow periods and high temperatures also had profound effects on soil processes to the interactive effect of these two factors on N mineralization (Cassman and Munns 1980), discussed below.

Soil N processes

In the HT system, RZ-SHAW tended to over-predict NO_3^--N content when soil moisture fell below 0.22 m^3 m^{-3}. Sharp declines in net N mineralization have been shown to occur at water suction levels between 0.3 and 2 bars at all temperatures (Cassman and Munns 1980). Although the soil temperatures were high in the HT system, this driver of soil microbial activity is overridden by limited soil moisture resulting in reduced decomposition of organic materials during fallow periods (Knewtson et al. 2012). Kumar et al. (1999) also noted poor prediction of water during the dry soil period may have led to improper simulations of N transformation processes of organic N, which in turn affected the simulations of soil NO_3^--N.

Further, fertilizer in the HT system was exclusively supplied from commercial pelletized organic fertilizers and horse manure compost. As some researchers have reported, N decomposition, denitrification, and nitrification processes are not predictable in soils with organic manure applied soil, as compared to soils with synthetic fertilizer applied (Hartz et al. 2000; Chen et al. 2013). Limited soil water content may also have led to discrepancies between the actual soil microbial growth and soil microbial community behavior manifested in the model algorithms (Ma et al. 2007).

The simulation estimated high daily N_2O fluxes in the HT system (> 90 g N_2O-N ha^{-1}) on four dates (April 22nd and 23rd in 2014, March 12th and September 25th in 2015) that did not correspond to field sampling events. Previous conclusions from the field experiment from this study hypothesized that despite relatively high NO_3^--N levels in the HT system that N_2O fluxes may be less than expected due to a high degree of control over soil moisture (Shrestha et al. 2019). However, this simulation effort indicates that the likelihood that peak flux levels were likely missed in routine sampling. Further study is needed to better understand N cycling in HT systems, including and that increased sampling rigor which is warranted and likely would have improved model fit in this study.

Discrepancies between simulated and observed soil NO_3^--N levels were observed primarily at the start of the simulation in the CONV and LI system. In the CONV system, plot management history included vegetables on raised beds with fertilizer added via irrigation lines (fertigation), leading to heterogeneous

soil disturbance and nutrient input patterns. As such, high variability in soil NO_3^--N content and N_2O flux in field replicates were observed and may indicate high spatial variability in soil NO_3^--N content in all three soil layers and during the initial year of the experiment (Fig. 5). However, RZ-SHAW effectively simulated soil NO_3^--N and N_2O during the remainder of the simulation, indicating model sensitivity to the residue and the tillage conditions at the initiation of the simulation.

The beginning of the simulation period in the LI system corresponded to the time period immediately after pasture conversion to vegetable plots. Prior to the first vegetable crop in the rotation (pepper), LI plots were maintained for five years with rotational grazing of cattle, enriched with heterogeneous distribution of cattle dung and urine. These large inputs with high spatial variability led to high variability in measured soil NO_3^--N and N_2O flux values, and conditions which RZ-SHAW could not accurately predict during the first month of the pepper crop. Further, initial pasture crop residue values were estimated, complicating fit issues early in the vegetable crop rotation.

Although the simulation did not accurately predict N_2O peak values after the pasture conversion by deep tillage, the model simulation did demonstrate large N_2O peaks and the general flux pattern observed in field measurements. Large N_2O peaks have been observed in other works upon incorporation of organic amendments including crop residues (Hansen et al. 2019; Pinto et al. 2004) as well as manure inputs (Heller et al. 2010; Deng et al. 2013). The mechanism for such N peaks following incorporation of large additions of organic amendments likely affects multiple model processes, such as N consumed in N_2O production also enhancing oxygen depletion by stimulating microbial respiration and promoting anaerobic conditions for denitrification (Chen et al. 2013; Hansen et al. 2019).

The effects of pasture conversion on N cycling identify opportunities for sustainable intensification in LI systems

Rotational pasture-crop systems have been posited as a sustainable farming system that optimizes food production and improvement of soil health (Franzluebbers and Gastal 2019; Grahmann et al. 2020). Such systems may minimize external inputs and

provide integration of crop and livestock production systems. The simulation results and observations of crop and soil management challenges provide opportunities for targeted inputs to that may increase yields with minimal environmental impact. The N mineralization rate in the LI system was substantially higher in the first year after conversion from pasture (0.6 kg N ha^{-1} day^{-1}) than the average for the rotation (0.4 kg N ha^{-1} day^{-1}), which led to high N leaching losses during the first year following pasture conversion. In addition to high leaching losses, simulation results showed further asynchrony between the crop N requirement and N availability in the LI system. After the first year in the rotation, crops suffered from nutrient stress at planting due to low levels of mineral soil N, leading to reduced crop growth and low yields in the LI system. Poor crop growth in the LI system also favored weed growth leading to lower crop yield and overestimation of simulated crop yields.

Additional organic N inputs applied at transplant may aid in crop establishment and competitiveness against weeds (Vann et al. 2017) with minimal N losses. Further, supplemental irrigation at key stages of crop establishment and drought stress may improve crop growth and yield. Finally, targeted weed cultivation to improve crop competition relative to weeds, offer opportunities to sustainably increase yields in this system (Vann et al. 2017).

Nitrate leaching is the dominant N loss pathway in diversified vegetable production systems

The main pathway of N loss was through NO_3^--N leaching in all systems (Table 7). Simulated cumulative NO_3^--N leaching from the soil profile was highest in the CONV system followed by LI and the HT systems. Despite model fit issues with soil NO_3^--N levels discussed previously, trends in measured and simulated values indicate lower N leaching losses than reported by other researchers. For example, Feaga et al. (2010) reported NO_3^--N leaching of 29–150 kg N ha^{-1} per year with single crop a year from broccoli and beans field with the application of 67–240 kg N ha^{-1}. The observed lower leaching losses in the CONV system, though higher than other systems in this study, may be lower than literature values due to (1) reduced amount of rainfall water entering into the soil plastic mulch that reduced the

Table 7 Model simulated cumulative N processes and losses from 2014 to 2016 in conventional (CONV), low input organic (LI), and organic high tunnel (HT) production systems

	Total N					
	Mineralization kg N ha^{-1}	Denitrification	Immobilization	Uptake	leaching	N fixation
CONV	465	49	26	694	158	61
LI	376	32	28	321	135	28
HT	1032	13	386	664	79	39

downward movement of rainfall water and (2) improved synchronization between N fertilizer application (with drip irrigation in split doses) and the crop N requirement. Despite relatively lower leaching levels, leaching losses were pronounced in the CONV and LI systems after the crop (pepper) harvest in 2014, as well as during the subsequent spring (March 2015). These periods correspond to periods of high rainfall, and lack of sufficient crop or cover crop biomass to uptake excess soil moisture and N.

Despite having a higher soil NO_3^--N content in the soil profile, less leaching loss of NO_3^--N was simulated in the HT compared to the CONV system mainly because of the prolonged dry fallow period and lacking the leaching effect of rainfall inside tunnels (Wang et al. 2018). Total soil N mineralization over the simulation period in the HT system was 2.1 times the values estimated for the CONV system, and 2.7 times the values estimated for the LI system (Table 7). However, as discussed below, reduced leaching losses in HT systems may be offset by heretofore unknown gaseous losses.

HT systems experience increased N mineralization rates, benefitting crop growth but creating soil management challenges

The average mineralization rate in the HT system was 1.18 kg N ha^{-1} day^{-1} with a maximum value of 3.60 kg N ha^{-1} day^{-1}, reflecting the consistently higher soil N mineralization in the HT system compared to LI and CONV systems. The average mineralization rate was 0.55 kg N ha^{-1} day^{-1} in the CONV system (with maximum rate of 2.45 kg N ha^{-1} day^{-1}) and in the LI system was 0.44 kg N ha^{-1} day^{-1} (with a maximum mineralization rate of 2.41 kg N ha^{-1} day^{-1}). Higher N

mineralization rate in the HT is due to higher soil temperature (Wang et al. 2019) and continuous availability of substrate supplied from compost and organic fertilizers applied prior to each crop. The immobilization rate in the HT system was very high just after the incorporation of horse manure compost but decreased sharply after a week and followed by increased N mineralization with increased soil moisture with drip irrigation. The continuous application of compost over the years causes nutrient loading and salt accumulation problems (Rudisill et al. 2015). Further, high mineralization rates and increased decomposition rates can lead to mineralization of the soil organic matter in HT systems (Wang et al. 2019), illustrating some of the challenges to sustainable soil management in these systems.

Denitrification losses were greater in open field systems utilizing synthetic fertilizers

Along with greater N leaching losses, the CONV system also demonstrated higher simulated cumulative denitrification N loss (49 kg N ha^{-1}) compared to the LI (32 kg N ha^{-1}) and HT (13 kg N ha^{-1}) systems (Table 7). Higher denitrification losses in the CONV system may be due to the high soil water content throughout the cropping period. Denitrification loss in the HT system was isolated to the crop growing season and lasted only 1–2 days, though denitrification peaks were larger than in the CONV and LI systems. Such pronounced periods of denitrification losses in the HT system may be due to soil drying and subsequent rewetting cycles, which elevates N mineralization and denitrification (Guo et al. 2014), though the process may be short-lived (Borken and Matzner 2009) and occur primarily during fallow periods between cropping periods.

Crop N uptake and yield underestimated in HT system

Crop yields were consistently underestimated in the simulation of the HT system, with the exception of the beet crop and bean crops. Crop yields may be greater in the HT system, on average, due to the protective microclimate of the HT structure. HT-grown crops have been found to have greater yields that field-grown crops due to decreased foliar disease pressure (O'Connell et al. 2012; Rudisill et al. 2015), control of the water level in the root zone due to rainfall exclusion and irrigation to optimize nutrient uptake and limit root pathogens (Rho et al. 2020), as well as decreased wind in the crop canopy (Rho et al. 2020), which allows for more vigorous crop growth and higher yields.

Despite this generally favorable microclimate for other crops, bean yields were very low in the HT system compared to open field systems despite having a high N uptake and vegetative growth. Lower yields were likely related to heat stress, which was observed in field measurements and accounted for in the RZ-SHAW simulation. Heat stress of more than 30 °C is critical to flowering and pod development in beans, resulting in significant reductions in pod number, seed number and seed weight as a result of abscission of buds and flowers and reduced pollen viability (Rainey and Griffiths 2005). Maximum air temperature inside the high tunnels were measured at more than 30 °C for 60 days of the total 71 days of growing period and were as high as 41 °C and during the flowering period. The model simulated this heat stress to the bean plants in the HT system through lower simulated pod numbers were very low in HT beans (80 pods m^{-2}), compared to the CONV systems (557 pods m^{-2}). As such, the HT bean plants accumulated higher biomass, but lower bean yield compared to CONV bean plants, and were terminated earlier (71 days after planting due to yellowing of plants) than the CONV beans (80 days after planting). Lower bean yield in the LI system may be attributed to weed pressure, which is not simulated. Early season weed control was sufficient for bean plants to establish and reach peak vegetative growth but could not compete with uncontrolled weeds during fruit setting. It should be noted that in the LI system beans were terminated after only two harvests (53 days after planting) due to weed competition.

Table beet yield and biomass were not simulated well by the model in any system, due in large part to the lack of an available table beet variety in the RZWQM2 crop growth module. A sugar beet crop growth module was used as an alternative, which matures to a considerably larger size and requires additional time to maturity than a table beet. Such crop morphology differences likely contributed to the lack of fit between simulated and measured values for beet crop yield, crop biomass, and soil N content. Similarly, the cabbage growth module was used to simulate collard growth. For both table beet and collard crops, plant parameters in the crop growth modules were modified using measured data or values from the literature. Additional modifications that were unsupported by measured or literature data were not modified for the sake of improving model fit.

Conclusions

The simulation results using RZ-SHAW have provided the better understanding of N dynamics and losses over time in diversified vegetable systems. As inputs and tillage intensity differed between these systems, so too do the opportunities to decrease N losses and sustainably intensify these systems. Our results suggest that N leaching losses may be minimized by reducing the amount of the basal (pre-plant) dose of fertilizer and increasing the number of (split) fertilizer applications in CONV production systems, as indicated by high soil moisture and simulated leaching values. In the LI system, pre-plant fertilizer and supplemental irrigation may increase the crop yield and reduce N losses by improving crop stand establishment. Although evaluating alternatives to full pasture inversion is beyond the scope of this study and simulation, the effect of this element of the rotation is pronounced and opportunities to explore how to reduce N losses appear warranted.

Despite effectively simulating the soil temperature and soil water conditions in the HT system, simulation results demonstrated inconsistencies in predicting soil NO_3^--N patterns in the upper soil layers, and precise N_2O flux values. This simulation effort highlights the potential for atypical soil microbial and other N-cycling processes to be occurring in HTs due to the unique microclimate, which warrants further study. Chiefly among these, increased sampling rigor must be

applied, particularly early in the cropping cycle and after significant perturbations, such as wetting events after prolonged drought. Overall, simulation and measured values demonstrated the potential for more efficient water and N fertilizer management strategies in each system. Future research utilizing RZWQM simulations to inform potential management scenarios may improve the efficiency of field research activities and provide opportunity to more sustainably intensify such diversified vegetable production systems.

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