

## Ontology-based simulation of water flow in organic soils applied to Florida sugarcane

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### ABSTRACT

An ontology-based simulation (OntoSim) is a unique data modeling environment where soil–plant–nutrient processes are represented as database objects and the user-defined relationships among objects are used to generate computer code (Java) for running the simulation. The aim of this study was to model hydrologic processes of sugarcane-grown organic soils utilizing OntoSim in the Everglades Agricultural Area (EAA) of South Florida. This OntoSim-Sugarcane model describes the complex hydrology of sub-irrigation and open ditch drainage commonly used on Florida farms.

Model calibration was conducted by (i) selecting rectangular farm water management units (<12 ha), which are encompassed with farm ditches, from two farms in the EAA, (ii) assembling all relevant input data including water tables (WT) recorded at the monitoring farm well of each unit, and (iii) optimizing the fits between the simulated and observed daily WT during two consecutive water years (WY). By calibrating two site-specific parameters – lateral saturated hydraulic conductivities of soil profiles and vertical saturated hydraulic conductivity of the underlying limestone bedrock – good agreement between simulated and observed daily WT was obtained (Nash–Sutcliffe efficiency coefficient >0.65; coefficient of residual mass <1%) within the units during WY96–97 (May 1995–April 1997). The validation of the model during subsequent WY98–99 at both units also showed Nash–Sutcliffe efficiency >0.55 and coefficient of residual mass <3%. It indicated that OntoSim-Sugarcane is able to simulate daily fluctuations of WT within the farm units and estimate lateral drainage/sub-irrigation and deep seepage that significantly contribute to the water balance at farms in the EAA. Thus, it can be a promising management tool to provide farmers with accurate assessment of water movement in this agricultural area.

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### 1. Introduction

The Everglades Agricultural Area (EAA), which is located between Lake Okeechobee and the Everglades Protection Area (EPA) in South Florida, has been established since late 1940s when an extensive flood-control system consisting of canals, ditches and water control structures was installed to convert wet or submerged historic Everglades into productive croplands (Snyder and Davison, 1994). Currently 200,000 ha of the EAA are cultivated and approximately 82% of the cultivated area is planted to sugarcane (*Saccharum officinarum* L.) followed by vegetables, rice

(*Oryza sativa* L.), and sod (Rice et al., 2002). Besides favorable environmental conditions including fertile organic soils (Histosols) and subtropical climate (Baucum et al., 2006), Florida sugarcane industries in the EAA have been sustained by seepage-based drainage control systems where farm water tables (WT) are managed to maintain the water level normally <1 m below the soil surface (Obreza et al., 1998). Such WT controls can be effective in the EAA due to the facts that (i) Florida has a flat topography (Snyder and Davison, 1994), (ii) its organic soils ranging from 0.30 to 3 m depth are underlain by an impermeable limestone bedrock (Snyder, 1994), and (iii) over half of the average annual rainfall (about 1360 mm y<sup>-1</sup>) falls during the wet season from June to October (Ali and Abtew, 1999).

While the sugarcane industry currently ranks third in Florida agricultural economy behind the greenhouse/nursery and citrus industries (Baucum et al., 2006) due to these water control

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systems, numerous studies have also shown their adverse effects on water quality in the EAA and downstream hydrologic units (e.g. LOTAC II, 1990; Izuno et al., 1991). Since Histosols in the EAA have been formed within a low-nutrient oligotrophic ecosystem that contains low quantities of essential plant nutrients except nitrogen, the soils often require fertilization for agriculture production (Luo, 2004). This agricultural practice combined with water control systems has contributed to nutrient enrichment of the Everglades by releasing phosphorus (P) enriched farm drainage water from the EAA to the EPA (Izuno and Bottcher, 1994; Sievers et al., 2003). Thus, there is a need to better optimize water management in the EAA considering its complex hydrology so as to reduce the environmental impacts associated with P fertilizer application and P-enriched farm drainage water. Several studies have been conducted to understand the hydrology of the EAA by using mathematical modeling (Bottcher et al., 1998; Zhang and Gornak, 1999), which is now widely employed by agronomists and environmental scientists to understand complex soil–plant–nutrient processes in various agroecosystems because unlike empirical approaches using statistical analyses of historical records it can be further applied to test management scenarios and predict responses to future changes in climate.

Currently, most mathematical simulations are implemented in a particular programming language like FORTRAN, C++, or Java, and provide graphical user interfaces to run simulations. However, there are multiple limitations to this traditional approach of simulation modeling. First, mastery of a programming language is required to develop and/or modify a simulation model. Second, documentation is physically separate from the model implementation and sometimes does not accurately describe the model implementation. Third, often written documentation of a simulation model does not capture all details of program code so that ultimately it is necessary to read computer code in order to truly understand how the model works (Beck et al., 2008). To overcome these limitations ontologies have received much attention for implementing mathematical models and building simulation systems in order to explicitly describe knowledge of a simulation model (Lacy and Gerber, 2004; Cuske et al., 2005).

Ontologies are formal representations of the concepts and their interrelationship within a particular domain (Beck et al., 2008). An application of ontologies to modeling and simulation results – *OntoSim* – has been presented by Beck et al. (2008). *OntoSim* provides a unique data modeling environment where the processes related to plant growth, soil moisture, and nutrient uptake are represented as database objects and relationships among objects are used to generate computer code (Java) for running the simulation. *OntoSim* was originally developed to help Florida citrus growers optimizing yields in an economically effective manner (Beck et al., 2008). However, *OntoSim* can provide a platform to develop any conceptual and mathematical simulation model.

This paper presents the use of *OntoSim* to model hydrology of sugarcane farms on organic soils in the EAA of South Florida. Main emphasis was made on modeling vertical and lateral drainage flux in the saturated zone to facilitate simulation of WT control systems commonly used on Florida sugarcane farms with sub-irrigation and open ditch drainage. Calibration and validation of these processes were conducted using farm data collected during a four-year period, followed by a discussion about future applications of *OntoSim* to other modeling environments.

## 2. Materials and methods

### 2.1. Ontology-based simulation applied to Florida sugarcane

Mathematical concepts and algorithms documented in forms of publications and simulation models were utilized to build

ontological implementations of water flux on sugarcane-grown farms resulting in a simulation model, called *OntoSim-Sugarcane*. The processes for soil organic matter decay were based on the mathematical framework of the CENTURY model (Parton et al., 1988). Soil–water uptake and transpiration of sugarcane for calculating evapotranspiration (ET) were described according a modified version of the DSSAT/CANEGRO model (Inman-Bamber, 1994; Inman-Bamber and Kiker, 1997). Hydrologic processes for simulating a perched WT and vertical and lateral drainage flux in the saturated zone were adapted from DRAINMOD (Skaggs, 1980) and other studies (Alexander, 1988; Reyes et al., 1993).

All the processes identified for simulating sugarcane growth on Florida organic soils have been represented as mathematical equations. Reverse engineering from program code into equations was conducted in cases where processes were found in the form of computer code from various models (e.g. DSSAT/CANEGRO). These equations have been represented as database objects of *OntoSim* using *SimulationEditor* and *EquationEditor* (Fig. 1a and b). First, to describe the topological and thematic structure of *OntoSim-Sugarcane*, five compartments – weather, soil profile and layer, and sugarcane and sugarcane stalk – were created using the structure editor, which is the main interface of the *SimulationEditor* (Fig. 1a). This tool provides functionalities which enable modeler to create and maintain a simulation project by designing the structure of a system (Beck et al., 2008). Then 195 equations and 247 symbols associated with the elements in the structure diagram were created using the *EquationEditor* (Fig. 1b), which uses an interface similar to other equation editors such as Microsoft Office Equation Editor, except that equations and symbols are stored internally as ontology objects. Then computer code (Java) to run a simulation is generated automatically from the equations and symbols. Finally, the simulation model was debugged for errors to run successfully.

### 2.2. The hydrologic processes for water table control systems in the EAA

The drainage systems in the EAA feature extensive networks of farm canals, ditches, and pump stations that are managed by both the South Florida Water Management District (SFWMD) and growers. The district manages the public canals and its own pump stations in the EAA while growers manage water levels on their farm drainage basins within the EAA basin. Normally, a main farm canal runs from the farm pump station to the far reaches of the farm, and sub-mains or farm laterals branch off the main canal at right angles, generally on 800 m spacing, on section and half section boundaries (Izuno, 1994). Emanating at right angles from the farm laterals are equally spaced field ditches, which are parallel and subdivide the farm into rectangular areas with nominal dimensions of 200 by 800 m. These 16 ha blocks are considered the basin water management unit where sub-irrigation or open ditch drainage practices are accomplished by either raising or lowering field ditch water levels (Izuno, 1994).

In this work, such concept of farm water management unit was adapted and a small farm unit (<12 ha) was selected from an entire farm area as the hydrologic modeling unit where the hydrologic processes, including continuous calculation of soil moisture contents, actual evapotranspiration (AET), upward water flux, infiltration, and drainage loss according to the water table simulated for each process, were simulated.

#### 2.2.1. Distribution of soil moisture

Water tables on fields underlain by a restrictive layer have been simulated by various hydrologic models such as DRAINMOD, ADAPT (Agricultural Drainage and Pesticide Transport) (Alexander, 1988), and GLEAMS-WT (Groundwater Loading Effects of Agricultural Management Systems–Water Table) (Reyes et al., 1993).

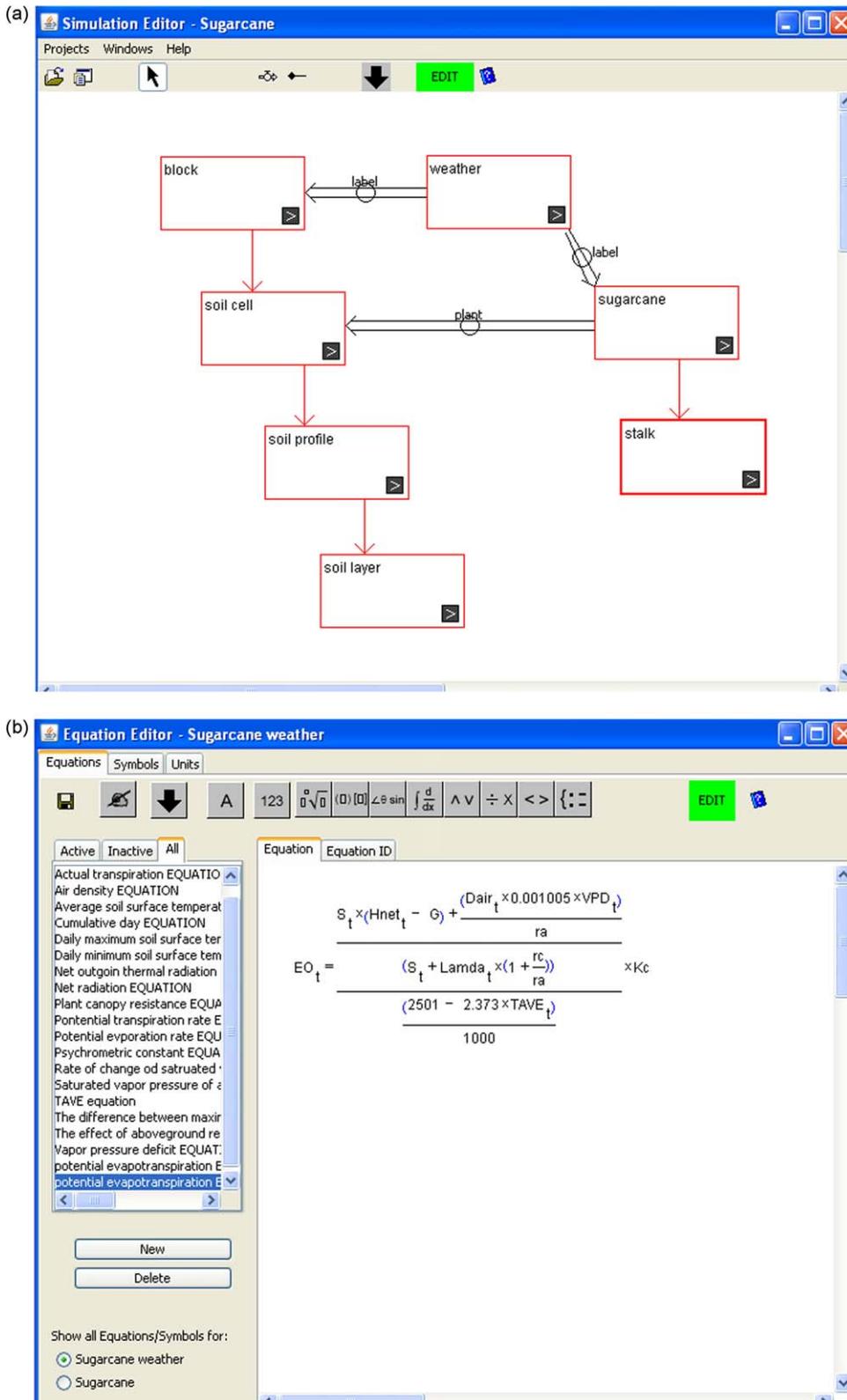


Fig. 1. The system structure of the OntoSim-Sugarcane and equations and symbols created using the SimulationEditor (a) and EquationEditor (b).

These models have a common feature that the soil moisture distribution within the soil profile is assumed to be at a “drained to equilibrium” condition. In this case, the moisture content for each soil layer can be defined by an empirical function that describes the soil–water characteristic relationship between soil–water content ( $\theta$ ) and the corresponding soil matrix potential ( $\psi$ ). The equation of Van Genuchten (1980) was adapted to estimate moisture

distribution within the soil profile:

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r) \left[ \frac{1}{1 + |\alpha\psi^n|} \right]^m \tag{1}$$

where  $\theta_r$  and  $\theta_s$  are the residual and saturated soil–water content ( $\text{cm}^3 \text{cm}^{-3}$ ), respectively;  $\psi$  is the soil matrix potential or capillary

pressure head (cm) that is equal to the distance from soil layer to a water table under hydrostatic equilibrium; and the empirical parameters  $\alpha$  ( $\text{cm}^{-1}$ ),  $n$  and  $m$  are estimated by the fitting of this function and the data measured for the soil–water retention relationship. Here it is assumed that  $m = 1 - 1/n$ . An example in Fig. 2a shows the distribution of soil moisture (curve A<sub>1</sub>–B<sub>1</sub>–C<sub>1</sub>) corresponding to the depth of WT below the soil surface (WTD<sub>1</sub>) in cm using Eq. (1).

### 2.2.2. Calculation of actual evapotranspiration and upward flux

The soil moisture distribution calculated is allowed to deviate from steady-state due to the removal of water from the profile by ET, resulting in a root zone depleted of water. This deviation implies that an upward gradient is induced between the water table and the depleted root zone and thus water may move upwards in the soil profile by upward flux in response to this gradient. This upward movement of water is estimated by assuming that a steady-state condition exists between the water table and an evaporating surface. A similar approach as presented by Martinez (2006) using the algebraic solution of Anat et al. (1965) was used to estimate maximum upward flux ( $U_{\text{FLUX}}$  in cm):

$$U_{\text{FLUX}} = VK_{\text{SAT}} \left( 1 + \frac{1.886}{\eta^2 + 1} \right)^\eta \left( \frac{\text{RD}}{h_b} \right)^{-\eta} \quad (2)$$

where  $VK_{\text{SAT}}$  is vertical saturated hydraulic conductivity ( $\text{cm h}^{-1}$ );  $\eta = 2 + 3n(1 - 1/n)$ ; RD is root zone depth (cm) that changes with time during the growing season and is determined by using the bottom of a root zone as the upper boundary; and  $h_b$  is often referred to as bubbling pressure (cm) and determined from the relationship between effective saturation and  $\psi$  (Skaggs, 1980).

The actual upward flux is taken as the smaller one of either  $U_{\text{FLUX}}$  or ET calculated as a function of potential ET [the FAO (Food and Agriculture Organization of the United Nations)-56 Penman–Monteith equation] (Allen et al., 1998) and model-simulated leaf area index and root length density (Jones et al., 2003).

If  $U_{\text{FLUX}}$  meets ET demand, actual upward flux is equaled to ET. This results in the increase of soil air volume (or the decrease of soil–water volume) by the upward flux within a soil profile, causing a new WT to recede from the previous WT. The new WT is estimated using the relationship between soil air volume within an entire soil profile and the new WTD. For example, the soil air volume for each layer, which can be calculated using Eq. (1) at specific WTD, is summed up within the entire soil profile to give specific total air volume at the specific WTD. By repeating this procedure, the relationship between soil air volume and various WTDs can be derived and modeled using a simple equation that can be used to estimate fluctuation of WT according to corresponding change of soil–water volume due to ET and drainage loss:

$$\text{AirV} = a_1 \text{WTD}^2 + a_2 \text{WTD} \quad (3)$$

where AirV is the air volume (cm) in the entire soil profile, and  $a_1$  and  $a_2$  are coefficients.

Accordingly, a soil moisture distribution is updated based on the new WTD and the moisture in the root zone can be still under a steady-state condition. The curve A<sub>2</sub>–B<sub>2</sub>–C<sub>2</sub> of Fig. 2b illustrates the case when  $U_{\text{FLUX}}$  meets ET demand and thus WTD<sub>1</sub> becomes WTD<sub>2</sub>.

If  $U_{\text{FLUX}}$  fails to meet ET demand, actual upward flux is equaled to  $U_{\text{FLUX}}$  and a new WTD is calculated using the same procedure as used for the previous case. But soil moisture in the root zone, deviates from a steady-state condition by the difference between ET and  $U_{\text{FLUX}}$ , creating a water depleted root zone. Fig. 2b shows a new moisture distribution in such case (curve D–E–B<sub>2</sub>–C<sub>2</sub>) corresponding to the new WTD (WTD<sub>2</sub>).

### 2.2.3. Infiltration

Infiltration rates are calculated by the equation of Green and Ampt (1911) simplified as

$$f = \frac{A}{F} + B \quad (4)$$

$$A = VK_{\text{SAT}}(\theta_s - \theta)h_b \left( \frac{\eta}{\eta - 1} \right) \quad (5)$$

$$B = VK_{\text{SAT}}$$

where  $f$  is the infiltration rate which is equal to the downward flux ( $\text{cm h}^{-1}$ );  $F$  is the cumulative infiltration ( $\text{cm h}^{-1}$ ); the parameters  $A$  and  $B$  depend on the soil properties, initial water content and distribution, and surface condition; and  $\theta$  is soil–water content at the corresponding WTD in this case. Thus, the relationship between  $A$  and  $B$  and WTD can be derived, resulting in estimated infiltration rates according to WTD.

Once infiltration rate is estimated, the amount of infiltration is compared with the depth of a depleted root zone within the soil profile. If it is greater than the infiltration, all soil layers are completely replenished to drained volume soil–water content and WTD is updated as a new WTD (WTD<sub>3</sub>, Fig. 2c) and the distribution of soil moisture follows hydrostatic equilibrium with the WTD. Otherwise, infiltration fills up the first soil layer and so on until no water is left for infiltration.

### 2.2.4. Water flux

Lateral drainage (water flux from farm to ditch), or sub-irrigation (water flux from ditch to farm), is calculated using WT of farm water management unit and farm ditches (Fig. 3).

$$Q_L = \frac{4K_e(WT_{\text{farm}} - WT_{\text{ditch}})[2(WT_{\text{ditch}} - d) + WT_{\text{farm}} - WT_{\text{ditch}}]}{S^2} \quad (6)$$

where,  $Q_L$  is either lateral drainage or sub-irrigation ( $\text{cm h}^{-1}$ );  $K_e$  is effective lateral saturated hydraulic conductivity ( $\text{cm h}^{-1}$ ) that is a function of lateral saturated hydraulic conductivity of the soil profiles ( $LK_{\text{SAT}}$ ) (Skaggs, 1980);  $WT_{\text{farm}}$  and  $WT_{\text{ditch}}$  (cm) are the WT at the farm water management unit and ditch above mean sea level (AMSL);  $S$  is the distance from the middle of a farm unit to the ditch (cm); and  $d$  is the distance from the bottom of ditch to the mean sea level (cm).

Deep seepage ( $Q_V$ ,  $\text{cm h}^{-1}$ ) from soil profiles to limestone bedrock, which is estimated by a straightforward application of Darcy's law, can be present if there are solution holes and fractures in the limestone bedrock.

$$Q_V = \frac{VK_{\text{SAT-bedrock}}(WT_{\text{farm}} - WT_{\text{ditch}})}{d_{\text{bedrock}}} \quad (7)$$

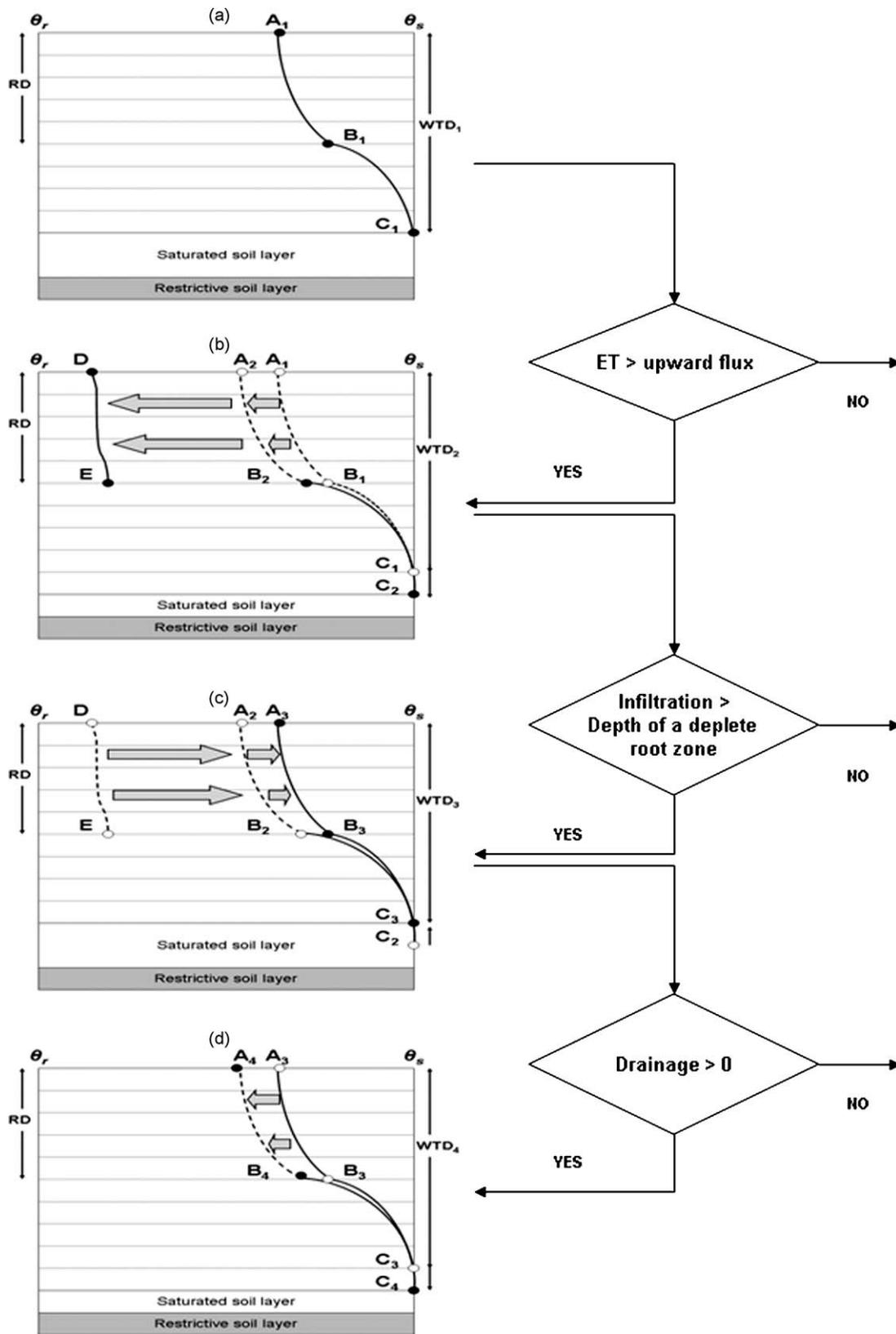
where  $VK_{\text{SAT-bedrock}}$  is vertical saturated hydraulic conductivity of the underlying limestone bedrock ( $\text{cm h}^{-1}$ ) and  $d_{\text{bedrock}}$  is its thickness (cm).

Fig. 2d shows the new water table (WTD<sub>4</sub>) receding from the previous water table as drainage decreases water content within the soil profile.

## 2.3. Model testing

### 2.3.1. Dataset

Two farms in the EAA where comprehensive best management practice (BMP) research has been conducted to monitor BMP implementation and related P load parameters from 1992 to 2002 (Daroub et al., 2009) were selected for this study. One farm, UF9202A, has an area of 130 ha under sugarcane monoculture. The average ground surface elevation is 388 cm AMSL and the average soil depth of its Lauderhill mucks (Euic, hyperthermic, shallow



**Fig. 2.** Flow chart of the hydrologic processes calculated in the OntoSim-Sugarcane: (a) the distribution of soil moisture (curve A<sub>1</sub>–B<sub>1</sub>–C<sub>1</sub>) corresponding to WTD<sub>1</sub> under “drained to equilibrium” condition; (b) the new moisture distribution (curve D–E–B<sub>2</sub>–C<sub>2</sub>) calculated when U<sub>FLUX</sub> fails ET demand (soil moistures in the root zone are deviated from a steady-state condition by the difference between ET and U<sub>FLUX</sub>, creating a depleted root zone); (c) the moisture distribution when all soil layers are completely replenished to soil–water content of hydrostatic equilibrium with the WTD<sub>3</sub>; (d) the moisture distribution corresponding to WTD<sub>4</sub> receding from WTD<sub>3</sub> as drainage decreases water content within the soil profile.

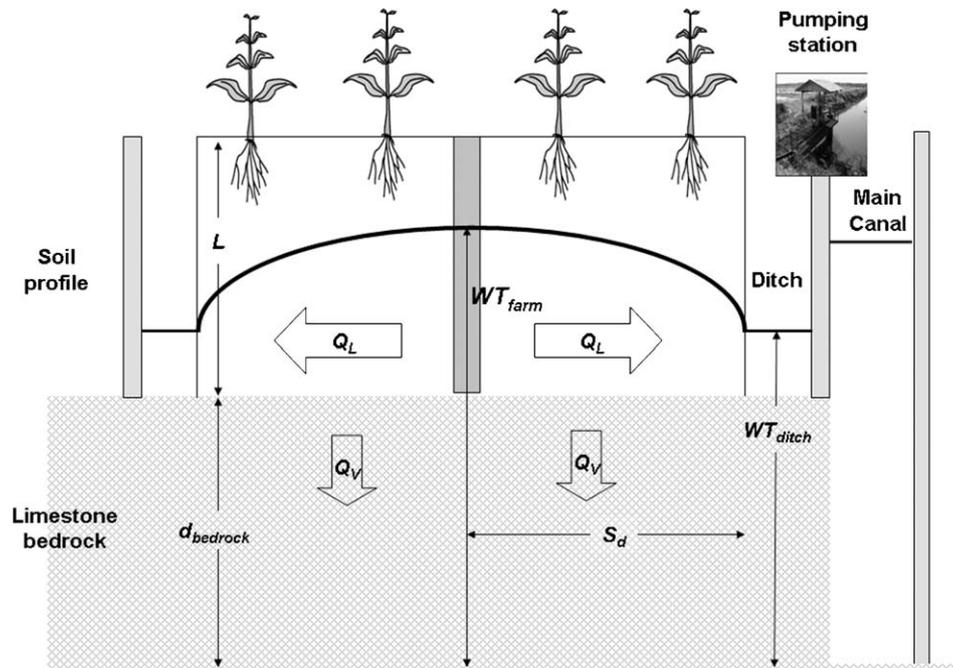


Fig. 3. Layout of the farm modeling unit used in this study.

Lithic Medisaprists) is about 46 cm (Garcia et al., 2001). The other farm site, UF9209A, has a size of 1244 ha under mostly sugarcane production and the average field surface elevation and Lauderhill/Pahokee mucks (Euic, hyperthermic Lithic Medisaprists) soil depth are 275 cm AMSL and 97 cm, respectively (Daroub et al., 2009). At farms, main farm canal levels, WT of several farm monitoring wells, rainfall, discharge flows, and discharge water P concentrations were monitored hourly from 1995 to 1999.

### 2.3.2. Model initialization and parameterization

The first step in running simulations for model calibration and validation was to specify the initial values of model state variables such as water content of each soil layer. One well-documented approach for model initialization is to conduct spin-up simulations prior to the period of the data record, which have been used to effectively eliminate the effects of assumptions about the initial values of state variables in various models (e.g. Paustian et al., 1992). Here, a one-year spin-

up simulation prior to the starting period for model calibration was utilized.

The soil parameters required for estimating soil moisture distribution (Table 1) were either directly obtained from the soil data of the Florida Soil Characterization Retrieval system (<http://flsoils.ifas.ufl.edu/>) or calculated by fitting the data with the equation of Van Genuchten (1980) at two soil profiles of each farm. Some of such calculated parameters were further used to estimate the relationship between air volume and WTD that is critical in calculating daily WT fluctuations. Daily temperature and total solar radiation, which are necessary to simulate daily sugarcane growth, were derived from Belle Glade weather station (about 17 km away from both farms) operated by the SFWMD.

Farm water management units in rectangular shape, which are about 7 ha (190 by 370 m) and 11 ha (140 by 800 m), were selected from farm UF9202A and UF9209A, respectively. Because a monitoring farm well was located at the approximate center of the farm unit, the WT records of the well were used in calculation

**Table 1**  
Main input parameters utilized for OntoSim-Sugarcane simulations of two farms (UF9202A and UF9209A) in the Everglades Agricultural Area.

Parameter	Value				Unit
	Farm UF9202A		Farm UF9209A		
<b>Soil</b>					
Depth ( $L$ )	50		88		cm
Distance from a farm well to a farm ditch ( $S_d$ )	9500		7000		cm
<b>Soil profile</b>					
	Upper	Lower	Upper	Lower	
Depth	0–25	25–50	0–45	45–88	cm
Saturated water content ( $\theta_s$ )	0.91	0.95	0.75	0.71	$\text{cm}^3 \text{cm}^{-3}$
Residual water content ( $\theta_r$ )	0.058	0.035	0.20	0.097	$\text{cm}^3 \text{cm}^{-3}$
Vertical saturated hydraulic conductivity ( $VK_{SAT}$ )	655	302	77	227	$\text{cm h}^{-1}$
Lateral saturated hydraulic conductivity ( $LK_{SAT}$ ) <sup>a</sup>	436	201	26	76	$\text{cm h}^{-1}$
Empirical parameter ( $\alpha$ ) used in the equation of Van Genuchten (1980)	0.01	0.0065	0.024	0.025	
Empirical parameter ( $n$ ) used in the equation of Van Genuchten (1980)	1.26	1.31	1.19	1.2	
<b>Limestone bedrock</b>					
$VK_{SAT-bedrock}$ <sup>a</sup>	0.045		0.015		$\text{cm h}^{-1}$
Thickness ( $d_{bedrock}$ )	75		84		cm

<sup>a</sup> Values were obtained from model calibration.

**Table 2**  
Statistical measures calculated for two farms during the periods of model calibration (WY96–97) and validation (WY98–99).

WY <sup>a</sup>	Farm UF9202A			Farm UF9209A				
	Number of observations	Statistical measure <sup>b</sup>			Number of observations	Statistical measure		
		DRMSE (cm)	CRM (%)	NSE		DRMSE (cm)	CRM (%)	NSE
96	365	6.55	-0.40	0.75	353	8.91	-0.47	0.60
97	357	6.14	1.86	0.55	346	7.14	0.54	0.73
96–97	722	6.35	0.71	0.69	699	8.08	0.02	0.66
98	365	6.20	0.03	0.26	347	10.19	1.26	0.65
99	365	3.63	-0.09	0.80	351	8.43	4.67	0.74
98–99	730	5.08	-0.03	0.57	698	9.35	2.94	0.69

<sup>a</sup> WY, water year.

<sup>b</sup> DRMSE, daily root mean square error; CRM, the coefficient of residual mass; NSE, the Nash–Sutcliffe efficiency coefficient.

of water flux. Farm ditch levels are also required to simulate lateral water flux in the units but are not often measured at typical farms in the EAA. Thus, in this study, main farm canal levels were utilized under the assumption that those would be good approximations of farm ditch levels. However, main farm canal depths are deeper than farm ditch depths because farm canals are often excavated into the underlying limestone bedrock while farm ditches are excavated to the bedrock. This difference can lead to lower water levels in the main farm canal than those in the farm ditch and thus in such cases, farm ditch levels were set to soil profile depth ( $L$ ). The thickness of the bedrock,  $d_{\text{bedrock}}$ , is approximated by the difference of the lowest water levels in the monitoring farm well excavated to the bedrock and the main farm canal. Some of the important parameters are shown in Table 1.

### 2.3.3. Model calibration and validation

Model testing included calibrating the model to a portion of the observed data and validating it using the remaining observations over four consecutive water years (WY). The WY period discussed herein begins May and terminates following April (Whalen and Whalen, 1996). The calibration was conducted by assembling all relevant input data for the two farm units and WT recorded at a monitoring well. These were simulated for WY96–97 (May 1995 to April 1997) and cross-checked with observed WT at the well for the same period (calibration phase). Because  $LK_{\text{SAT}}$  of two soil profiles and  $VK_{\text{SAT-bedrock}}$  were site-specific parameters, they were calibrated to give the best fit of the simulated and observed WT ( $WT^{\text{sim}}$  and  $WT^{\text{obs}}$ ). To quantify fits, the daily root mean square error (DRMSE) was utilized. It calculates an estimate of average absolute error in the units of the observed and predicted ones:

$$\text{DRMSE} = \sqrt{\frac{1}{i} \sum_{t=1}^i (WT_t^{\text{sim}} - WT_t^{\text{obs}})^2} \quad (8)$$

where  $i$  is number of observations and  $t$  is daily time steps.

After completing calibration of the model, validation was also conducted for the consecutive WY98–99 period (May 1997 to April 1999).

In addition to DRMSE, two more statistical measures were used to quantify the simulation results obtained from model calibration and validation. One is the coefficient of residual mass (CRM) that expresses the relative size and nature of the error (Singh et al., 2006):

$$\text{CRM} = \left( \frac{\sum_{t=1}^i WT_t^{\text{sim}} - \sum_{t=1}^i WT_t^{\text{obs}}}{\sum_{t=1}^i WT_t^{\text{obs}}} \right) 100 \quad (9)$$

Another valuable metric that describes the quality of model fits is the Nash–Sutcliffe efficiency coefficient (NSE) (Nash and Sutcliffe, 1970):

$$1 - \frac{\sum_{t=1}^i (WT_t^{\text{sim}} - WT_t^{\text{obs}})^2}{\sum_{t=1}^i (WT_t^{\text{obs}} - WT_t^{\text{obs}})^2} \quad (10)$$

where  $\overline{WT^{\text{obs}}}$  is the average of  $WT^{\text{obs}}$ . The NSE compares the differences between the daily simulation results and observations to the variance in the data. The NSE has a maximum value of 1.0 for a perfect fit model and zero for a model that is no better than the mean of the observations. The NSE can also take on negative values for very poor models.

## 3. Results

### 3.1. Model calibration and validation

When model parameters –  $LK_{\text{SAT}}$  and  $VK_{\text{SAT-bedrock}}$  – were manually calibrated to minimize DRMSE between daily  $WT^{\text{sim}}$  and  $WT^{\text{obs}}$  at rectangular water management units of the two farms over WY96–97, different sets of parameter values were obtained from the two farms. However, the  $LK_{\text{SAT}}$  of upper and lower soil profile can be calibrated proportional to  $VK_{\text{SAT}}$  but are lower than  $VK_{\text{SAT}}$  (Table 1). These findings are reasonable because  $LK_{\text{SAT}}$  is often estimated as based on the magnitude of  $VK_{\text{SAT}}$  and also it may be different by a factor of 10 (Skaggs, 1980). Non-zero  $VK_{\text{SAT-bedrock}}$  was required to get the lowest DRMSE at both farms, indicating that there were solution holes or fissures in the underlying limestone bedrock. Both  $LK_{\text{SAT}}$  and  $VK_{\text{SAT-bedrock}}$  of UF9202A were much higher than those of UF9209A (Table 1).

The DRMSE for model calibration during WY96–97 (Table 2) were 6.35 and 8.08 cm, respectively, which are approximately one tenth of the entire soil depths. At both farms, DRMSE was higher in WY96 than WY97 because larger amount of rainfall during WY96 induced more fluctuation of farm WT and resulted in larger discrepancy between daily  $WT^{\text{sim}}$  and  $WT^{\text{obs}}$  (Table 3). The CRM of both UF9202A and UF9209A ranged from negative to positive values with the average of <1% for the calibration period (Table 2). Because the CRM was used to measure the tendency of the model to overestimate or underestimate the observed values (Rasse et al., 2000; Singh et al., 2006), it can be concluded that OntoSim-Sugarcane model slightly overestimated the daily  $WT^{\text{obs}}$  overall. The NSE for both farms were >0.65 (Table 2) that are comparable to other studies where simulation of hydrologic flows such as subsurface drainages received NSE between 0.50 and 1.0 (Helweg et al., 2002; Wang et al., 2006). Figs. 4a and 5a display good agreement between daily  $WT^{\text{sim}}$  and  $WT^{\text{obs}}$  for the calibration period ( $R^2 = 0.74$  and  $0.63$  for UF9202A and UF9209A respectively).

Using the parameter values acquired from model calibration, the hydrologic processes were validated for the subsequent WY98–99 (Figs. 4b and 5b). The average DRMSE of validation was similar to that of calibration regardless of farms, whereas the CRM of validation increased or decreased within 3% based on farms (Table 2). This suggests that OntoSim-Sugarcane was sufficiently robust to model hydrologic processes across the two sugarcane farms. Unlike UF9209A, the NSE of UF9202A for the model validation was worse as indicated by a low NSE in WY98 (0.26) which was lowest among

**Table 3**

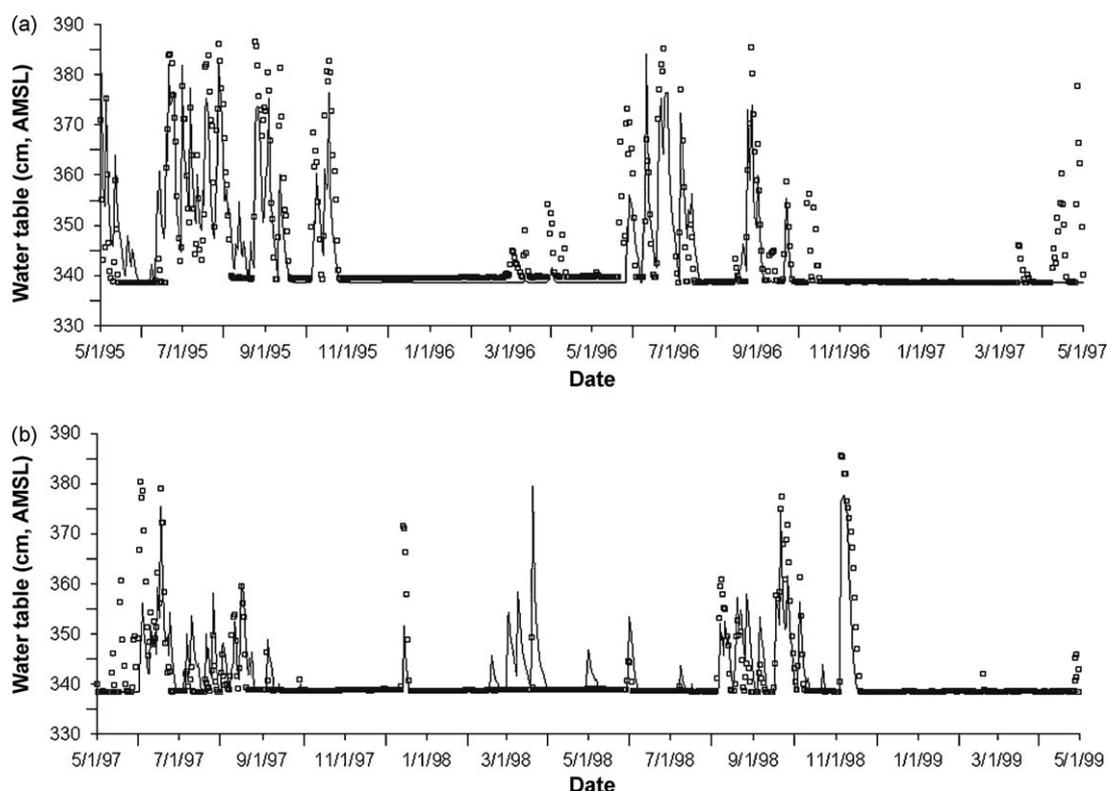
Water balance calculated for farm UF9202A and UF9209A based on the simulation results of model calibration (WY96–97) and validation (WY98–99). Values in the parenthesis indicate the percentage of each variable in the input or output.

	WY <sup>a</sup>	Input		Output			Net change <sup>c</sup> (mm)
		Precipitation (mm)	Sub-irrigation (mm)	ET <sup>b</sup> (mm)	Vertical seepage (mm)	Lateral drainage (mm)	
Farm UF9202A	96	1339 (99)	14 (1)	682 (47)	456 (31)	320 (22)	-105
	97	1120 (99)	10 (1)	880 (69)	220 (17)	174 (14)	-144
	98	1457 (100)	1 (0)	854 (73)	213 (18)	109 (9)	282
	99	941 (99)	9 (1)	709 (68)	196 (18)	142 (14)	-97
Farm UF9209A	96	1303 (72)	494 (28)	720 (40)	448 (25)	650 (35)	-21
	97	1255 (67)	622 (33)	921 (49)	387 (20)	586 (31)	-17
	98	1356 (76)	420 (24)	790 (45)	350 (20)	601 (35)	35
	99	1010 (63)	604 (37)	760 (46)	370 (23)	514 (31)	-30

<sup>a</sup> WY, water year.

<sup>b</sup> ET, evapotranspiration.

<sup>c</sup> Net change = input – output.



**Fig. 4.** Comparison of observed (blank circle) and simulated (solid line) daily WT for model calibration (a) and validation (b) at farm UF9202A.

the entire period of calibration and validation (Table 2). Such low NSE was partly due to overestimation of ET during the period from late WY97 to early WY98 and thus the model failed to match  $WT^{obs}$  with  $WT^{sim}$  (Table 2). In fact, it was assumed that sugarcane continued to be cropped during the entire period of calibration based on typical cropping practices in this region. However, there is a possibility of no sugarcane crop during the period and if such possibility is considered and reduced ET is applied to the period, the NSE could be improved to  $>0.45$  in WY98 at UF9202A. For other periods of validation, close agreement between daily  $WT^{sim}$  and  $WT^{obs}$  were observed as well ( $R^2 = 0.56$  and  $0.68$  for UF9202A and UF9209A respectively).

These calibration and validation results confirmed that the model is able to describe hydrologic process and the complex system of water control structures used at Florida sugarcane farms reasonably well by adjusting several model parameters regardless of soil depths of farms.

### 3.2. Water balance

Based on the simulation results of model calibration and validation, water balance at the farm unit was calculated for the entire simulation period (Table 3). Although surface runoff is typically considered as an output of water balance, it was assumed to be negligible at these farms due to rapid  $VK_{SAT}$  and the flat topography within the farms. Thus, precipitation and sub-irrigation from farm ditches were considered as water inputs while farm drainages and ET were treated as water outputs.

A wide range of annual precipitation (from about 900 to 1500 mm) was observed at the two farms during the four WY periods (Table 3). Such annual precipitation comprised almost all the total water input into UF9202A, but due to large amount of sub-irrigation, it was at most 76% of total water input at UF9209A. In terms of water outputs, the percentage of ET in the water losses was about 40–70% at both farms and the rest was lateral drainage

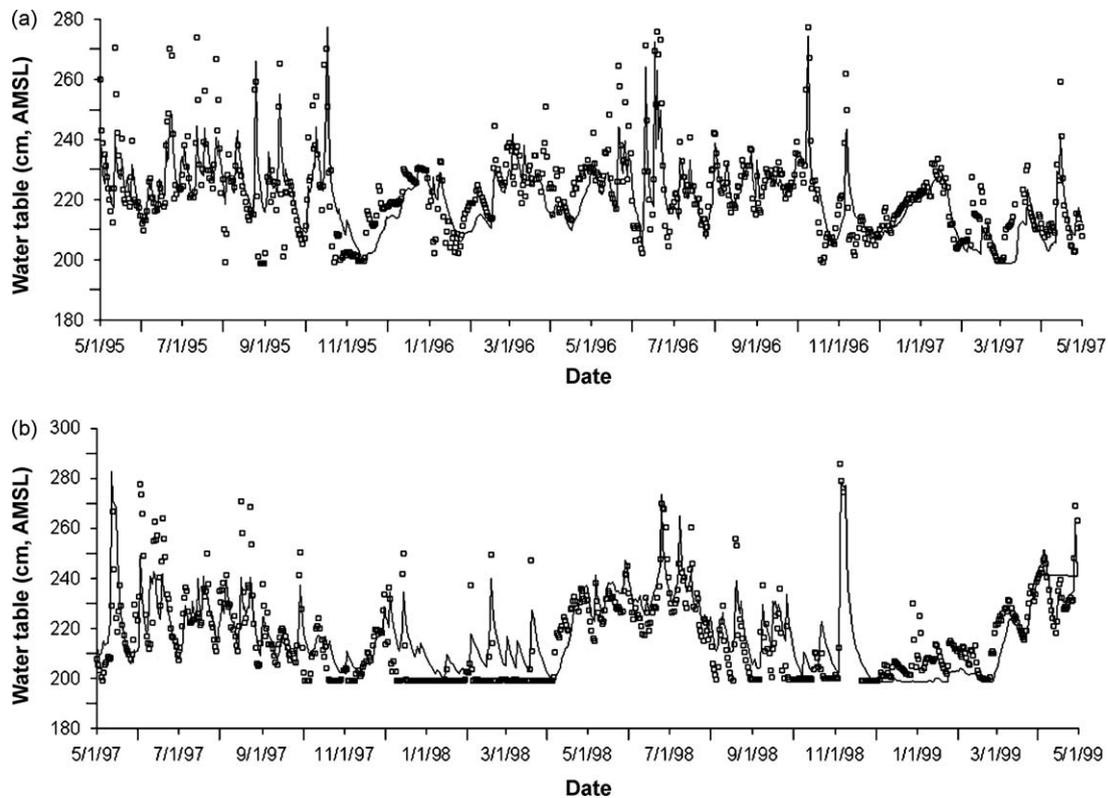


Fig. 5. Comparison of observed (blank circle) and simulated (solid line) daily WT for model calibration (a) and validation (b) at farm UF9209A.

and deep seepage that would be induced by an intensive WT control conducted at both farms.

## 4. Discussion

### 4.1. Water flux within farms

Because hydrologic/water management is the major variable controlling nutrient loads exported from the EAA (Grunwald et al., 2009), the ability to model drainage behavior is critical to assess the impact on nutrient influx from EAA farm drainage basins along ditches and canals into the EPA. As shown in this study, the two farms modeled here are strongly affected by lateral drainage and/or sub-irrigation due to intensive pumping activities. However, such results are based on the parameter values obtained from model calibration and thus findings from other similar studies conducted in EAA or low-relief drainage basins should be compared with the results reported here.

In fact, the BMP dataset used here has been used in many studies (e.g. Rice et al., 2002) mostly focusing on P loads. But one study by Garcia et al. (2001) has been conducted to analyze the pattern of drainage in six representative farms across the EAA including the farm UF9202A and UF9209A used to calibrate and validate OntoSim-Sugarcane. In their study, WT response to rainfall and drainage was characterized using four different types of rainfall events from the farms in order to empirically describe drainage events and calculate site water budgets. Overall, they found that (i) farm drainage behavior to channel gradients was not apparent and (ii) drainage rates measured in farm monitoring wells showed no direct relationships to distances across the farm or to the main station pumping rate, whereas model simulation showed that drainage rates can be properly modeled as a function of the gradient between the WT in the farm well and those in the ditches and the distance from a farm well to a farm ditch [Eqs. (6) and (7)]. This discrepancy might be because mathematical

approaches can handle all the complex processes at the same time while empirical approaches are more limiting. For example, WT response is affected by not only rainfall or pumping activities but also by deep seepage and ET at the same time.

Although it did not focus on farm drainage, the study of Chen et al. (2006) would provide important information about drainage pathways. Because the pathway of drained waters from farms to farm canals affects ion concentrations or specific conductance (an indirect measure of the total concentration of ions) in the drainage water, the information on ionic compositions or concentrations might be utilized to further verify the simulation results. Their study showed that (i) specific conductance in the EAA canals is strongly influenced by the composition of the shallow groundwater, historically reported to be high in  $\text{Na}^+$  and  $\text{Cl}^-$  due to connate seawater entrapment and (ii) the mixing of surface water and groundwater. Although the concentrations of several ions such as  $\text{Cl}^-$  were close between the two farms (Chen et al., 2006), the concentrations of  $\text{HCO}_3^-$  in the farm canals showed a significant difference between UF9202A (about  $280 \text{ mg L}^{-1}$ ) and UF9209A (about  $190 \text{ mg L}^{-1}$ ). Deep seepage in contact with limestone bedrock would contribute significantly more  $\text{Ca}^{2+}$  and  $\text{HCO}_3^-$  in the field canal waters, but if farm canal waters are sub-irrigated to farms, such concentrations will be reduced. This might explain lower concentrations of  $\text{Ca}^{2+}$  and  $\text{HCO}_3^-$  in the farm canals of the UF9209A where sub-irrigation was a significant source of water input (Table 3). This confirmed that the simulation well describes the water management of the two farms.

### 4.2. Future application of OntoSim to agriculture

As shown in this study, OntoSim has the potential to elevate modeling of systems in agriculture to a level of abstraction at which model building is no longer a software engineering problem, rather it becomes a knowledge representation problem in which reasoners can be applied to automatically classify, compare, and

search for models and model elements (Beck et al., 2008). The first steps have been taken in this direction by building an environment for constructing models and representing equations and symbols in a formal ontology language, and the utility of the approach was demonstrated by building a moderately complex model of soil, water, and nutrient management using this environment.

Furthermore, OntoSim can be used to build a database of models that can help to classify different but similar models which can be searched to locate models and model components suitable for various applications (Beck et al., 2008). Currently many different yet similar models to simulate soil–plant–nutrient processes in agriculture are available for model developers and general users. One reason for the diversity of models is the diversity of environments in which models need to be applied. There are hundreds of crops grown commercially, and while their physical and biological systems share commonality, there is variability of climate and geography as well as individualized crop characteristics that require different model implementations. However, having so many different yet similar models cause problems in managing models and in sharing model components among developers. There is unnecessary redundancy resulting from poor communication among developers. For example, they may use similar ways of calculating processes such as ET, or they may use different equations to achieve the same results. Unfortunately the traditional methods for creating these models make it very difficult to compare the models to see how they are similar or different.

In OntoSim, each specific model can be represented by an instance and abstract model structure and processes represented as classes. Similar models can be grouped together into a class, and related classes grouped together to form superclasses. At the top of the resulting taxonomy would be generic modeling. If an ontology is also used to represent the internal structure of a model, then model internals can be compared in an automated fashion to determine which parts of the models are similar and which are different. The vast collection of models and model components resulting from this analysis would create a large but organized taxonomy. This taxonomy could be searched using query processors based on ontology reasoners to locate models and model components of interest. It can also be used to compare and contrast two models and explicitly identify how they are different or similar. Although OntoSim–Sugarcane was adapted to modeling hydrologic processes in sugarcane, classes that describe infiltration or other, can be used in multiple other crop simulation models.

## 5. Conclusion

As a new modeling environment, OntoSim was utilized to model hydrology on organic soils in Florida sugarcane production where WT control systems have played an important role in nutrient enrichment of the Everglades by releasing P enriched farm drainage water from the EAA. Mathematical concepts of sugarcane growth and hydrologic processes were implemented into the OntoSim as database objects. Java computer code used to run the simulation was generated automatically from equations and symbols, in order to simulate an impermeable layer in the soil profile to model a perched water table and vertical and lateral drainage flux in the saturated zone.

By calibrating two site-specific parameters – lateral saturated hydraulic conductivities of two soil profiles and vertical saturated hydraulic conductivity of the underlying limestone bedrock – good agreement between simulated and observed farm WT was obtained (NSE > 0.65; CRM < 1%) within the farm units during WY96–97. Model validation during WY98–99 of WT at both farm units also showed good agreement between simulated and observed WT (NSE > 0.55; CRM < 3%).

Thus, OntoSim–Sugarcane presented here is able to simulate daily water tables within the farms and estimate lateral drainage/sub-irrigation and can be a useful tool to provide farmers with more accurate assessments of water managements on the area. Because OntoSim–Sugarcane can provide transparency of modeling processes, which is adaptable for multiple other applications, reusability of classes to model water movement in EAA can be used to model water movement elsewhere while other processes such as perched WT are specific to geographic landscape settings.

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