# Modeling of Phosphorus Loads in Sugarcane in a Low-Relief Landscape Using Ontology-based Simulation

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Water flow and P dynamics in a low-relief landscape manipulated by extensive canal and ditch drainage systems were modeled utilizing an ontology-based simulation model. In the model, soil water flux and processes between three soil inorganic P pools (labile, active, and stable) and organic P are represented as database objects. And user-defined relationships among objects are used to automatically generate computer code (Java) for running the simulation of discharge and P loads. Our objectives were to develop ontology-based descriptions of soil P dynamics within sugarcane- (Saccharum officinarum L.) grown farm basins of the Everglades Agricultural Area (EAA) and to calibrate and validate such processes with water quality monitoring data collected at one farm basin (1244 ha). In the calibration phase (water year [WY] 99-00), observed discharge totaled 11,114 m3 ha-1 and dissolved P 0.23 kg P ha-1; and in the validation phase (WY 02-03), discharge was 10,397 m<sup>3</sup> ha-1 and dissolved P 0.11 kg P ha-1. During WY 99-00 the root mean square error (RMSE) for monthly discharge was 188  $m^3$   $ha^{\mbox{--}1}$  and for monthly dissolved P 0.0077 kg P  $ha^{\mbox{--}1};$ whereas during WY 02-03 the RMSE for monthly discharge was 195 m<sup>3</sup> ha<sup>-1</sup> and monthly dissolved P 0.0022 kg P ha<sup>-1</sup>. These results were confirmed by Nash-Sutcliffe Coefficient of 0.69 (calibration) and 0.81 (validation) comparing measured and simulated P loads. The good model performance suggests that our model has promise to simulate P dynamics, which may be useful as a management tool to reduce P loads in other similar low-relief areas.

Copyright © 2010 by the American Society of Agronomy, Crop Science Society of America, and Soil Science Society of America. All rights reserved. No part of this periodical may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopying, recording, or any information storage and retrieval system, without permission in writing from the publisher.

J. Environ. Qual. 39:1751–1761 (2010) doi:10.2134/jeq2009.0509 Published online 28 July 2010. Received 23 Dec. 2009. \*Corresponding author (kwon.hoyoung@gmail.com). © ASA, CSSA, SSSA 5585 Guilford Rd., Madison, WI 53711 USA IN LOWLAND RIVER BASINS where flat topography and low hydraulic gradients are prominent, increased P loads from point/nonpoint sources have caused water quality and environmental degradation by accelerating eutrophication, altering ecosystem structure, and decreasing biodiversity in a variety of regions (Sharpley et al., 1996; Carpenter et al., 1998; Rabalais et al., 2002). Since the mid–20th century, such deterioration has spread rapidly from localized to large-scaled areas (Rabalais et al., 2002), such as the Gulf of Mexico where P flux from the Mississippi River Basin (2.9 million km<sup>2</sup>) has degraded coastal water quality (Rabalais et al., 2002; Alexander et al., 2008), and the Greater Everglades (8250 km<sup>2</sup>) where P influx from agriculturally dominated drainage basins (Everglades Agricultural Area) and urban areas have contributed to P enrichment (Izuno et al., 1991; Izuno, 1994).

Tracking of point and diffuse sources contributing to P enrichment in lowland river basins are confounded by the complexity of hydrologic pathways that occur as surface runoff, lateral or vertical flow in the vadose zone, or channelized in the form of drains, channels, or ditches. Drainage systems that accelerate flow in lowland systems have been optimized for agricultural production but have raised concerns about disproportionate, off-site nutrient enrichment. Pieterse et al. (2003) quantified the importance of sources of P and N in a lowland basin with high water table in the Netherlands and Belgium, and Foster et al. (2003) investigated suspended sediment and particulate P loads and pathways in lowland agricultural watersheds in the United Kingdom that have been altered by implementation of drains accelerating flow and transport patterns. In a multiscale study in a lowland, grasslanddominated watershed in the United Kingdom, the contribution of P to river transfers was investigated by Wood et al. (2005), who found that diffuse sources of P contribute at least 60% of the annual P flux without any significant inputs of P from river channel banks. In Florida, lowland river tributaries, agricultural

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Abbreviations: BMP, best management practice; CERES, Crop Environment Resource Synthesis; DSSAT, Decision Support System for Agrotechnology Transfer; EAA, Everglades Agricultural Area; NSE, Nash–Sutcliffe efficiency; SOM, soil organic matter; SWAT, Soil and Water Assessment Tool; TDP, total dissolved phosphorus; WT, water table; WY, water year.

production, and urbanization have given rise to major concerns about P enrichment impacting low-lying drainage endpoints (e.g., wetlands) (Grunwald and Reddy, 2008) or coastal areas (Perry, 2008). Trend analysis of nutrient concentrations and loads in four canals of the southern Indian River Lagoon showed significant increases (median total P in canals of 138 to 376  $\mu$ g L<sup>-1</sup>) exceeding USEPA ambient water quality criteria for the study area (Qian et al., 2007).

To address the problem of water quality degradation, best management practices (BMPs) have been suggested with the aim of reducing the impact of P loads from agricultural areas on natural ecosystems using either statistical analyses of water quality data (Grunwald et al., 2009) or mathematical modeling. The latter has been widely utilized due to its capability to test alternative BMP and predict their responses to future climatic changes in a fast and cost-effective way. A few examples include the use of the Soil and Water Assessment Tool (SWAT) (Arnold et al., 1998; Neitsch et al., 2002) to model riverine nutrient export from an east-central Illinois watershed to the Gulf of Mexico (Hu et al., 2007) and simple simulation models to assess the effects of various BMPs on P loads in EAA (Bottcher et al., 1998; Stuck et al., 2001).

However, there are some limitations inherent to such "traditional" simulation modeling such as the requirement of mastery of a programming language in developing and/or modifying a simulation model and ease of reuse of formalized knowledge. To overcome these limitations, ontologies have been used for implementing mathematical models and building simulation systems to explicitly describe knowledge of a simulation model (Lacy and Gerber 2004; Cuske et al., 2005) since the early 1990s. An ontology is defined as a formal, explicit specification of a shared conceptualization within a particular domain (Studer et al., 1998) on the basis of earlier definitions by Gruber (1993) and Borst et al. (1997). Formal refers to the fact that the ontology should be machine readable and explicit means that the type of concepts used, and the constraints on their use, are explicitly defined. Shared reflects that ontology should capture consensual knowledge accepted in the scientific communities, and conceptualization refers to an abstract model of phenomena in the world by having identified the relevant concepts of those phenomena (Studer et al., 1998). Smyth (1998) and Davis (1990) suggest domain-specific ontologies that are based on the following ontological elements: (i) content/entities, (ii) time, (iii) geometry, (iv) physics, and (v) logic. These ontological components, in turn, can be modeled computationally as objects, spatial or temporal representations, numerical models, or knowledge-base systems, and inference systems, respectively. Van Ittersum et al. (2008) present a component-based framework for agricultural systems (System for Environmental and Agricultural Modeling Linking European Science and Society, SEAMLESS) to assess agricultural and agrienvironmental policies and technologies across a range of scales (field to region), as well as some global interactions. The ontology-based framework links individual model and data components, and the software infrastructure allows a flexible reuse and linkage of components. Other ontology-based applications were focused on potato processing (Haverkort and Verdenius, 2006) and water quality (Chau, 2007). Beck et al. (2010) illustrated an ontology-based simulation model (OntoSim) of complex soilplant–nutrient processes represented as database objects and user-defined relationships among objects to generate computer code (Java) for running the simulation.

Kwon et al. (2010) used OntoSim to simulate daily fluctuations of water table (WTs) and estimate lateral drainage/ subirrigation and deep seepage that significantly contributed to the water balance within sugarcane farm basins in the lowland tributary of EAA. The model calibration and validation showed good agreement between simulated and observed daily WT with the Nash-Sutcliffe efficiency coefficient (NSE) (Nash and Sutcliffe, 1970) larger than 0.55 on two EAA farm basins. This study builds on OntoSim applied to EAA sugarcane farms (OntoSim-Sugarcane) that was extended to incorporate P transport and transformation processes. Our objectives were to: (i) develop ontology-based descriptions of soil P dynamics encapsulated into OntoSim-Sugarcane, and (ii) calibrate and validate simulations of P loads simulated by OntoSim-Sugarcane with water quality monitoring data collected in a low-relief EAA in south Florida.

# **Materials and Methods**

# **Description of Modeled Area**

The EAA of south Florida (Fig. 1), which was a submerged wetland of the oligotrophic Greater Everglades (Noe et al., 2001), was established by installing an extensive system of canals, ditches, and farm pump stations beginning in the late 1940s (Diaz et al., 1993). Since then, farm WTs have been effectively controlled either by pumping off excess water of individual farm basins into basin drainage canals of the EAA, or vice versa, because of Florida's flat topography (Snyder and Davidson, 1994). The EAA is a low-relief system with elevations ranging from 2.3 to 8.4 m above mean sea level (Fig. 1), organic soils underlain by impermeable limestone bedrock (Snyder, 1994), and affluent rainfall (~1270 mm yr<sup>-1</sup>) (Daroub et al., 2009). These ideal landscape conditions facilitated EAA to become one of the largest agricultural areas of organic soils for sugarcane production in the United States (Anderson, 1990). Currently, 200,000 ha of EAA are cultivated and approximately 82% of the cultivated area is planted to sugarcane followed by vegetables, rice (Oryza sativa L.), and sod (Rice et al., 2002).

Individual farm basins of EAA commonly feature: (i) main pump station, (ii) main farm canal, (iii) farm laterals, and (iv) farm ditches (Fig. 2). At the pump station, the water levels of a main farm canal are controlled either by off-farm discharge pumping from the main farm canal into the basin drainage canal operated by the South Florida Water Management District or by irrigated waters from the basin drainage canal to the main farm canal (Fig. 2). The main farm canal runs from the main farm pump station to the far reaches of the farm basin. Farm laterals are branched off the main canal at right angles and farm ditches are emanated at right angles from the farm laterals. These networks of laterals and ditches create rectangular areas (~16 ha) that are considered the basin water management unit where subirrigation or open ditch drainage practices are accomplished by either raising or lowering main farm ditch levels (Izuno, 1994). Such farm water management units were adopted as "a modeled area" where soil-plant-nutrient processes are simulated using OntoSim-Sugarcane. For this study we selected a modeled area (16 ha) of one EAA farm basin (farm UF9209A, 1244 ha) (Fig. 2) that was used in the previous calibration work of hydrologic processes (Kwon et al., 2010).

## Description of OntoSim–Sugarcane

### Modeled Processes

### Hydrology

In OntoSim–Sugarcane, soil moisture content is calculated using van Genuchten's (1980) equation where the soil-water characteristic relationship between soil-water content and the corresponding soil matrix potential is described under the assumption that the soil moisture distribution within the soil profile is at a "drained to equilibrium" condition. Evapotranspiration and infiltration are estimated by the Penman-Monteith equation (Allen et al., 1998) and Green and Ampt's equation (Green and Ampt, 1911), respectively. Lateral drainage (water flux from farm to ditch), or subirrigation (water flux from ditch to farm), is calculated using lateral hydraulic conductivity of soil profiles and the gradient between WTs of farm water management unit and farm ditches (Kwon et al., 2010). Vertical drainage from the soil profile to the underlying limestone bedrock is estimated by a straightforward application of Darcy's law. Finally, on-farm drainages calculated when WT of farm ditches are lowered by pumping activities to discharge excess water from the main farm canal into the basin drainage canal are considered as off-farm discharges.



Florida Department of Environmental Protection (original scale 1:24,000; Date:1999) Digital Elevation Model, U.S. Geological Survey/National Elevation Dataset (30m resolution)

Fig. 1. The elevation map of the Everglades Agricultural Area located in the state of Florida.

### Sugarcane Growth and Phosphorus Uptake

Simulation of sugarcane growth and P uptake is implemented using algorithms from widely known models. OntoSim-Sugarcane uses mathematical equations from the CANEGRO sugarcane model (Inman-Bamber, 1994) of the Decision Support System for Agrotechnology Transfer (DSSAT) (Jones et al., 2003) that was first developed from the Crop Environment Resource Synthesis- (CERES) Maize model (Jones and Kiniry, 1986) and was subsequently altered to integrate it into the DSSAT suite of models with further modifications (Singels and Bezuidenhout. 2002; Bezuidenhout et al., 2003; Singels et al., 2005). Daily sugarcane growth is simulated using tiller density (also known agronomically as stalk population), dry matter accumulation, partitioning of dry matter into aerial parts and roots, root growth, and water uptake. The tillering process is conceptualized as a series of cohorts emerging in concert with leaves on mother shoots and described using a polynomial function of thermal time. Then the resulting tiller density is used to model leaf area index and light interception,

which are parameters influencing photosynthesis (dry matter accumulation) and evapotranspiration (Bezuidenhout et al., 2003). Dry matter partitioning between root and aerial dry mass is simulated using a series of empirical equations according to Singels and Bezuidenhout (2002).

Sugarcane P uptake is estimated using findings reported in Coale et al. (1993) where nutrient accumulation patterns in the aerial portion of sugarcane were studied on organic soils of EAA. Combining their empirical equations of daily dry matter accumulation and P uptake, we calculated that an average of 0.95 kg P is accumulated in a ton of dry matter ha<sup>-1</sup>. This value is applied both to aerial and root P uptake of sugarcane.

#### Soil Phosphorus Dynamics

Three soil inorganic P pools—labile, active, and stable P—are modeled according to the equations developed by Jones et al. (1984) and Sharpley et al. (1984). The labile P includes fertilizer P, if any, and has potential of leaching or serves as P available to plant uptake. It is assumed to be in rapid equilibrium (days/weeks) with the active P, whereas the active P is in slow equilibrium with the stable P. The equilibrations among inorganic P pools are governed





#### Fig. 2. The layout of farm UF9209A located in the Everglades Agricultural Area.

by the P availability index that specifies the fraction of fertilizer P, which is in solution after the rapid reaction period.

Soil organic P dynamics is closely linked to C cycling derived from the CENTURY soil organic matter (SOM) model (Parton et al., 1988), where metabolic and structural fractions of surface and buried plant residues, and three primary SOM pools (active, slow, and passive) are modeled. P flows between SOM pools through soil mineralization/immobilization and are calculated as a function of the product of C flow rates, the C:P ratios for new decomposition products, and labile P content (Metherell et al., 1993). The leaching of soil labile P is modeled by assuming that a specific percentage of labile P is apt to be leached by drainage.

## Process Implementation Utilizing OntoSim-Sugarcane

Soil–plant–nutrient processes are implemented within OntoSim–Sugarcane as knowledge representations derived either from published algorithms that describe hydrology, nutrient transformation or transport processes, and crop cycling, or computer source codes of simulation models. An example is shown in Fig. 3a where the interaction between two inorganic P pools published by Jones et al. (1984) can be obtained either from their original publication or from the FORTRAN code of SWAT.

Then the overall model structure is specified in the form of elements created by the SimulationEditor that is a tool providing functionalities enabling a modeler to create and maintain a simulation project (Beck et al., 2010). We created five elements-weather, soil profile, soil layer, sugarcane, and sugarcane stalkto describe the topological and thematic structure of OntoSim-Sugarcane (Fig. 3b). The EquationEditor is used to define processes and symbols appearing in the algorithms associated with the model element (Fig. 3c). The EquationEditor uses an interface that resembles other equation editors such as Microsoft Office Equation Editor with the difference that the EquationEditor represents all the processes and symbols by using ontology objects (Beck et al., 2010). It is composed of three subeditors: Symbol Editor, Mathematical Expression Editor, and Unit Editor. Variables related to each equation are defined as symbols using the Symbol Editor, whereas the process in itself is defined as the relationship among symbols. Although the processes obtained in the form of mathematical equations can be entered into the model

without much modification, reverse engineering, i.e., the step converting from program code into equations, is required in cases where processes were found in the form of computer codes (Fig. 3c). Finally, the SimulationEditor automatically generates Java computer code to run simulations and generate output (Fig. 3d).

# **Model Testing for Phosphorus Loads in the EAA Farm Basin** Model Simulation

Most parameters related to SOM dynamics and sugarcane growth were set as default values specified by the original



Fig. 3. Overview of process implementation utilizing OntoSim–Sugarcane.

models such as CENTURY and DSSAT/CANEGRO (Table 1). Model variables such as initial soil C:P ratio were determined on the basis of bulk soil C:P ratio reported on several muck soils of EAA (Martin et al., 1997). Parameters 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 van Genuchten's (1980) equation at two soil profiles of a farm. Two hydrologic parameters - lateral saturated hydraulic conductivities of soil profiles and vertical saturated hydraulic conductivity of the underlying limestone bedrock - were obtained from the calibration work previously conducted at the farm during WY 96-97 (Kwon et al., 2010). Farm canal water levels and rainfall continuously recorded at the main farm pump station of the farm basin were also used.

Once all parameters were derived, OntoSim–Sugarcane was used to run the simulation for consecutive water years from May 1998 to April 2003 (WY 99–04) when at least 85% of farm basin UF9209A was cropped to sugarcane. Importantly, daily off-farm discharges and labile P loads transported from the modeled area (see description of modeled area) to the basin drainage canal by the discharges were simulated and expressed in m<sup>3</sup> ha<sup>-1</sup> and kg P ha<sup>-1</sup>.

### Model Calibration and Validation

Calibration of P processes is ideally conducted by comparing the data of dissolved P loads observed at the modeled area with labile P loads simulated by OntoSim–Sugarcane. However, such observations have not been recorded at the modeled area of this low-relief farm basin. Instead, total P and dissolved P loads (the product of daily discharge volume with the flow composite P concentration associated with the discharge event) have been recorded at the main farm pump station whenever

Table 1. Ke	y model parameters re	guired for simulating	hydrology and soil	P dynamics using On	ntoSim–Sugarcane at farr	n UF9209A.

Parameter		lue	Unit	
Farm modeled area				
Area			ha	
Distance from a farm well to a farm ditch	10,000		cm	
Thickness of limestone bedrock beneath soil	84		cm	
Soil profile	Upper	Lower		
Depth	0–44	44-88	cm	
Saturated water content	0.75	0.71	cm <sup>3</sup> cm <sup>-3</sup>	
Residual water content	0.20	0.097	cm <sup>3</sup> cm <sup>-3</sup>	
Lateral saturated hydraulic conductivity†	154	454	cm h⁻¹	
Decay coefficient of an active soil organic matter pool	7.3		<b>yr</b> <sup>-1</sup>	
Decay coefficient of a slow soil organic matter pool	0.2		<b>yr</b> <sup>-1</sup>	
Decay coefficient of a passive soil organic matter pool	0.0044		<b>yr</b> <sup>-1</sup>	
Initial C:P ratio	1,500			
A percentage of a simulated inorganic labile P pool that is leached by drainage‡	5		%	
Limestone bedrock				
Vertical saturated hydraulic conductivity†	0.015		cm h⁻¹	
Sugarcane				
P uptake	0.95		kg P ton of dry matter <sup>-1</sup>	

‡ Calibrated in this study

#### Table 2. Summary of data recorded at farm UF9209A.

Water year (WY)†	Discharge	Total P	Dissolved P	Particulate P‡
	m <sup>3</sup> ha <sup>-1</sup>		kg P ha <sup>-1</sup>	· · · · · · · · · · · · · · · · · · ·
99	4,253	0.58	0.12	0.46
00	6,861	0.36	0.11	0.25
99–00	11,114	0.94	0.23	0.71
02	4,199	0.10	0.04	0.06
03	6,198	0.24	0.07	0.17
02–03	10,397	0.34	0.11	0.23

+ Water year starts May and ends the following April.

‡ Particulate P is determined as the difference between total P and dissolved P.

the off-farm discharge pump was activated (Table 2). Because of the homogeneous nature of the studied farm basin in terms of soils, parent material, and land use management, we used the following stepwise approaches. First, we normalized the observed discharge values at the main farm pump station of the farm basin (1244 ha) to unit area discharges (m<sup>3</sup> ha<sup>-1</sup>) and then compared them to the simulated ones obtained at the modeled area of 16 ha. The same approach was used to compare observed dissolved P loads with simulated labile P loads.

To minimize the objective function of RMSE between monthly observed and simulated P loads that are calculated from summing up daily values, we manually adjusted one parameter—the percentage of a simulated labile P pool that can be leached by drainages during two consecutive water years, WY 99–00. After completing model calibration, simulation runs extended for three consecutive years (WY 01–03) and WY 02–03 were taken for model validation. We omitted the data of WY 01, leaving a one WY gap between model calibration and validation due to lower rainfall (<980 mm) than other WYs (>1170 mm).

The NSE was used as an additional statistical measure to quantify the fits between simulated and observed P loads,

NSE = 
$$1 - \frac{\sum_{i=1}^{i} (S_i - O_i)^2}{\sum_{i=1}^{i} (S_i - \overline{O_i})^2}$$
 [1]

where O and S are observed and simulated P loads;  $\overline{O}$  is the average of O; *i* is number of observations; and *t* is time step.

# **Results and Discussion**

## Simulation of Farm Discharges

The comparison between monthly simulated and observed discharges is summarized in Table 3. The simulated discharges were derived by summing up daily vertical and lateral drainages simulated during the days when off-farm discharge pump was activated. During the four WYs we studied the monthly RMSE evaluating discharge, which ranged from 176 to 214 m<sup>3</sup> ha<sup>-1</sup> (calibration and validation phases). Slightly higher RMSE was observed for WY 02–03 than for WY 99–00, despite lower discharge volumes due to the largest discrepancy of monthly discharge during September 2001 (WY 02) (Fig.

4b). NSE measures the relative magnitude of the residual variance to the variance of the observations (maximal NSE = 1) and indicates how well the observations and predictions fit a 1:1 line. NSEs were greater than 0.70 for discharge, regardless of WY. The maximum NSE for drainage achieved was 0.91 for WY 00. These values were comparable to those reported in other studies utilizing hydrologic models. For example, Singh et al. (2006) obtained 0.65 to 0.91 as NSE for their calibration work of DRAINage MODel (Skaggs, 1980), where monthly subsurface drainages for Iowa's tile landscapes were simulated. Another study by Santhi et al. (2001) suggested that the calibration and validation of SWAT for simulating monthly surface runoff and base flow for watersheds in Texas is satisfactory if NSE is greater than 0.60. Considering all these values, NSEs obtained from this study indicate good fits between simulated and observed discharges.

Further comparison was made between cumulative simulated and observed discharges (Fig. 4a and b). The difference between the two was small with 840 m<sup>3</sup> ha<sup>-1</sup> representing 7.5% of the total cumulative observed discharge for WY 99–00, which decreased up to 93 m<sup>3</sup> ha<sup>-1</sup> accounting for 0.9% of the total cumulative observed discharge for WY 02–03.

These results suggest that the hydrologic processes simulated at the modeled area (16 ha) are representative of those observed at the entire farm basin (1244 ha). This can be attributed to: (i) this farm basin has flat topography, and (ii) the internal booster pump installed at approximately two-thirds of the way down the length of the main farm canal successfully contributed to the uniformity of farmwide WT.

## Simulation of Soil–Plant Dynamics of Phosphorus

To validate the simulated results related to soil–plant P interactions, we compared modeled soil net mineralization and sugarcane uptake rates with literature values obtained from studies in this area.

For the WYs simulated here, the modeled rates of soil net P mineralization ranged from 29 to 40 kg P ha<sup>-1</sup> yr<sup>-1</sup> (calibration and validation phases). There have been several studies to measure net mineralization rates with laboratory leaching experiments on organic soils of south Florida in Pakokee muck (Euic, hyperthermic Lithic Haplosaprists). Reddy (1983) observed the total amount of mineralized P during 350 d of soil incubation under ambient temperatures and periodic leaching. The

Water year (WY†)	Мо	nthly discharge‡		Mon	thly dissolved P‡	
	No. of observations	RMSE	NSE§	No. of observations	RMSE	NSE
		m³ ha-1			kg P ha⁻¹	
99	12	188	0.83	11	0.0086	0.58
00	9	187	0.91	8	0.0067	0.78
99–00	21	188	0.86	19	0.0077	0.69
02	9	214	0.71	9	0.0024	0.79
03	12	176	0.83	11	0.0020	0.84
02–03	21	195	0.78	20	0.0022	0.81

+ Water year starts May and ends the following April.

‡ Monthly values are calculated from summing daily values.

§ NSE, Nash-Sutcliffe efficiency coefficient.

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Fig. 4. Comparison of simulated and observed off-farm discharges for (a) model calibration and (b) validation at farm UF9209A. Symbols and lines indicate monthly values (observed: closed mark; simulated: open mark) aggregated by summing up daily values and cumulative values (observed: solid line; simulated: dotted line), respectively.

amount measured was 4 µg P cm<sup>-3</sup> of soil, which is equivalent to 36 kg P ha<sup>-1</sup> yr<sup>-1</sup> if 90 cm soil depth is applied to the rate calculation. A much higher rate was estimated by Diaz et al. (1993), whose laboratory leaching experiments were conducted using a constant temperature (25°C). About 32 kg P ha<sup>-1</sup> yr<sup>-1</sup> was estimated within 15 cm soil depth resulting in 192 kg P ha<sup>-1</sup> yr<sup>-1</sup> based on 90 cm soil depth. Because the model accounts for the effects of soil temperature and moisture on SOM decay, Reddy's assessment would be more plausible – matching more closely with the rate derived from OntoSim–Sugarcane simulations. This close agreement might also indicate that default SOM decay coefficients worked well for this area.

Most of mineralized P was modeled as uptake by sugarcane (24 to 32 kg P ha<sup>-1</sup> yr<sup>-1</sup>) when we applied P uptake rates of above-ground biomass measured by Coale et al. (1993) for calculating P concentrations in both above-ground and below-ground biomass. This may be obvious because most crops act as P sinks in agricultural systems. It should be noted that there is uncertainty in estimating root P uptake because we used the same P uptake rate of root biomass as aerial P uptake rate. In fact, any kind of assumptions on root P uptake in models are biased because of spatial-temporal dynamics that are difficult to measure and are still poorly understood (Smith et al., 2005). However, such uncertainty in correctly estimating root P uptake rate should not be overemphasized in modeling total dissolved phosphorus (TDP) loads where the variations of root P uptake are less sensitive when compared to accurately simulating discharge activities and P fertilization movements.

## Simulation of Phosphorus Loads by Farm Discharges

Given the homogenous soil-hydrology conditions across the studied farm basin, which was confirmed by field observation, we proceeded to model P processes across the entire farm basin. By manually calibrating the percentage of a simulated labile P pool that is leached by drainage (Table 1) to minimize RMSE between monthly sums of daily simulated labile P loads and observed dissolved P loads for the period of WY 99–00, the RMSE of 0.0077 kg P ha<sup>-1</sup> and NSE of 0.69 were obtained (Table 3 and Fig. 5a). Both statistical measures were much lower in WY 99 than in WY 00 because there was large discrepancy between simulated and observed TDP during WY 99. As shown in Fig. 5a, dissolved P recorded in January 1999 was 0.026 kg P ha<sup>-1</sup>. Labile P loads simulated in January 1999 were less than one-tenth of the observed P loads resulting in the



Fig. 5. Comparison of simulated labile P and observed dissolved P loads for (a) model calibration and (b) validation at farm UF9209A. Symbols and lines indicate monthly values (observed: closed mark; simulated: open mark) aggregated by summing up daily values and cumulative values (observed: solid line; simulated: dotted line), respectively.

largest distinct difference between the two. When we removed the possible outlier, NSE was improved to ~0.89.

Model validation using the calibrated parameter value for WY 02–03 showed comparable value of NSE (0.81) to that obtained from WY 00 (Table 3). This can be explained by closer NSE between simulated and observed discharges in the validation period than in WY 00. In addition, this is consistent with findings that discharge volume is the major controlling variable to predict P loads in EAA (Stuck et al., 2001; Grunwald et al., 2009). Overall model performance on simulating P loads can be considered successful if the same NSE criteria as discharge simulations are applied. Considering that modeling errors in discharge propagate into routines to model P loads, the validation results of the latter confirm that simulations performed well.

Unlike NSE, much lower RMSE was obtained for the validation period than for the calibration period due to significant reduction of dissolved P loads that could be confirmed by comparing cumulative P loads seasonally. Simulated P loads showed the same pattern as observed P loads over WY with an apparently significant reduction of cumulative P loads from 0.23 kg P ha<sup>-1</sup> for WY 99–00 (Fig. 5a) to 0.11 kg P ha<sup>-1</sup> for WY 02–03 (Fig. 5b). Because soil P mineralization and sugarcane P uptake were not significantly different during the two periods on the basis of our model results, we can conclude that such decrease can be attributed to no or less P fertilization and lower discharge amount for the latter period. In fact, a slow P accumulation in sugarcane for several months following fertilizer application has been observed by Izuno et al. (1991), which could induce loss of applied P from the root zone during the early portion of the growing season if subsequent field drainage occurred following heavy rainfall events. The effect of P fertilization on total P loads has been documented in the EAA study by Daroub et al. (2009). Mixed crop farms showed either decreasing or insignificant trends in total P loads after 7 to 10 yr of implementing mandatory BMPs, whereas sugarcane farms showed a decreasing trend. The insignificant trends can be attributed to fertilization in vegetable crops, such as lettuce (Lactuca sativa L.), sweet corn (Zea Mays L.), and green beans (Phaseolus vulgaris L.), grown periodically as a rotation crop between sugarcane crops, which receive up to 150 kg P ha-1 (Castillo and Wright 2008). This suggests that the greatest potential for reducing P loads in EAA may be achieved by optimized P fertilization rates and improved drainage practices (Izuno et al., 1991).

A similar pattern was also found for total P data where total P loads showed a remarkable decrease from 0.94 kg P ha<sup>-1</sup> to 0.34 kg P ha<sup>-1</sup> (Table 2) due to the reduction in P input by management practices controlling floating aquatic vegetation growth, including mechanical harvesting and chemical spraying. Unlike other areas where particulate P is transported into surface water during surface runoff (Sharpley et al., 2002), a significant fraction of particulate P in EAA originates from in-stream biological growth rather than from field soil erosion (Stuck et al., 2001). Thus, further modeling efforts should be made to model complex processes inside canals where P immobilization and remobilization of sediments occur depending on interevent times and hydrodynamic conditions.

## **Summary and Conclusions**

As we demonstrated using error assessment and trend comparisons, OntoSim–Sugarcane successfully simulated monthly P loads by discharges at one sugarcane farm basin in EAA. Because the important features of the farm basin – flat topography, relatively uniform soil depths, and extensive artificial drainage systems – are similar to other sugarcane-grown farm basins in EAA (>160,000 ha), the model may have the potential to simulate P loads in other sugarcane farms of EAA.

OntoSim–Sugarcane has been developed to model P dynamics in sugarcane in organic soils as demonstrated in this study. It could also be applied to model P dynamics on adjacent sugarcane farm basins on sandy soils bordering EAA where approximately 20% of the sugarcane in Florida is grown (Gilbert et al., 2008). Furthermore, OntoSim–Sugarcane can offer benefits to adapt a given simulation model to different landscape settings since process knowledge is encapsulated in the form of database objects and user-defined relationships among objects. These objects can be modified, reused, shared, and enhanced as new process knowledge becomes available with much more ease when compared to legacy, hand-coded, simulation models.

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