Parameterization, Verification, and Validation of a Physiologically Complex Age-structured Rice Simulation Model

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ABSTRACT

A model of rice (Oryza sativa L.) growth and development is presented which accurately simulates the seasonal numbers and mass of roots, culms, leaf sheaths, leaf blades, panicle vegetative components, and grains for the main tillers and sub-tillers. The physiological detail imbedded within the model departed to the greatest degree from previously published rice simulation models in its tiller cohort and plant part age structure, and its metabolite partitioning structure. Possibly the greatest distinction between RICEPSM and previously developed rice models is the inclusion of a statistically rigorous model parameterization, verification, and validation process. The verification-validation approach used in this paper has the advantage of enabling the individual and collective fit of multiple response variables. The verified model explained 88% of the variability across 13 data types, with 88 and 93% of the variability explained for main tiller and sub-tiller grain yield, respectively. When validated against a second year of data, 87% of the variability across the 13 data types, and 92 and 95% of main tiller and sub-tiller grain yield, respectively, was explained. The paper contrasts the verification and validation approach presented in this paper with that used in other simulation-based papers. © 1997 Elsevier Science Ltd. All rights reserved

INTRODUCTION

A number of rice simulation models have been developed (van Keulen, 1978; Angus and Zandstra, 1980; McMennamy and O'Toole, 1983; Huang and Wang, 1986; Ritchie et al., 1987; Costello et al., 1988; Zhang and Chen, 1990; Graf et al., 1990b; Miller et al., 1993; Salam et al., 1994; Singh and Padilla,

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1995). These models represent a range of approaches to analyzing the response of rice to physical, agronomic, and biotic factors. Perhaps the most detailed rice model, RICEMOD was developed by McMenamy and O'Toole (1983). The objective of this model was to describe the complex biochemical and biophysical systems interacting in a rice crop. In contrast to RICEMOD and the other models listed above, Graf *et al.* (1990b) developed a rice model that uses a demographic and metabolic pool approach which is based on earlier models developed by Gutierrez and co-workers (Gutierrez and Wang, 1976). Although this model captures less physiological detail, it contains an age structure, a characteristic which facilitates evaluating the impact of physical and abiotic stresses on rice growth, development, and yield, and linking plant models with herbivore, pathogen, nematode, and weed population models.

The value of a simulation model is in part dependent on its ability to realistically mimic targeted response variables. Initially parameterized models frequently fail to accurately fit data from which the models were at least in part developed. To correct this situation, some parameters or functions are adjusted within biologically reasonable limits, and the new model output is again compared with the dependent data. This process is called model verification. In contrast, validation is the comparison of output from a verified model with independent data, followed by statistical analyses that test the degree of fit. Without a statistically rigorous validation, a verified model represents little more than a sophisticated curve-fitting and does not enable a statement of certainty as to its ability to capture a crop's response to major physical, agronomic, and biotic variables.

The goal of this paper is to use an analytical approach to quantify the response of rice to major physical variables. The approach presented comprises development of a model which combines the features of a physiologically complex model with an age-structured model. We parameterize the model, herein referred to as RICEPSM (**RICE** Population Simulation Model), using data obtained from the literature and field experiments. The ability of RICEPSM to capture the response of rice to major physical (i.e. daily maximum and minimum temperatures, and solar radiation) and agronomic variables (i.e. planting date, amount and timing of nitrogen applications, first day of permanent flooding, and plant density) is then tested using a rigorous statistically based parameterization–verification–validation procedure.

MATERIALS AND METHODS

Data sources for model parameterization

Table 1 summarizes the data sources used to parameterize RICEPSM. To estimate parameters that were not available through the literature, and to

TABLE 1
Data Sources for Parameterizing the Physiologically-Based Rice Population Model

Process	Unit	Regulating variable	Unit	Data source
Supply				
Photosynthesis	$\mu \text{ mol CO}_2 \text{ s}^{-1} \text{ m}^{-2}$	Hourly solar radiation	$\mu \text{ Einstein s}^{-1} \text{ m}^{-2}$	Tanaka <i>et al.</i> (1966), Yoshida (1981) Bouhache and Bayer (1993) Huang <i>et al.</i> (1990) Dingkuhn <i>et al.</i> (1990) Model simulation Same
		Hourly temperature	$^{\circ}\text{C}$	
		Leaf nitrogen	N% of mass	
		LAI	None	
		Supply/demand (S/D)	None	
Nitrogen uptake	$\text{g N m}^{-2} \Delta t^{-1a}$	Root surface areas	$\text{m}^2 \text{ g}^{-1} \text{ root mass}$	
		$\text{NH}_4^+ - \text{N}$	$\text{g} [\text{NH}_4^+ - \text{N}] \text{ m}^{-3}$	Youngdahl <i>et al.</i> (1982)
Demand				
Maintenance respiration	$\text{g} [\text{CH}_2\text{O}] \text{ m}^{-2} \text{ h}^{-1}$	Hourly temperature	$^{\circ}\text{C}$	Liang <i>et al.</i> (1986)
Growth respiration	$\text{g} [\text{CH}_2\text{O}] \text{ m}^{-2} \text{ At}^{-1}$	Mass and types of structures	g m^{-2} , none	Okano <i>et al.</i> (1984)
Grains	$\text{g} [\text{CH}_2\text{O}] \text{ or N m}^{-2} \Delta t^{-1}$	Net photosynthesis	g m^{-2}	Yoshida (1981)
Panicle branches	Same	No. of grain, growth rate	Grains m^{-2} , g grain $^{-1} \text{ At}^{-1}$	Panicle tagging data 1993
Leaf blades	Same	No. of branch, growth rate	Branches m^{-2} , g branch $^{-1} \text{ At}^{-1}$	Same
Culms	Same	No. of blade, growth rate	Blades m^{-2} , g blade $^{-1} \Delta t^{-1}$	Leaf tagging data 1992
Leaf sheaths	Same	No. of culm, growth rates	Culms m^{-2} , g culm $^{-1} \text{ At}^{-1}$	Same
Roots	Same	No. of sheath, growth rate	Sheathes m^{-2} , g sheath $^{-1} \Delta t^{-1}$	Same
Reserve	Same	No. of root, growth rate	Roots m^{-2} , g root $^{-1} \text{ At}^{-1}$	Same
		Growth demand	$\text{G} [\text{CH}_2\text{O}] \text{ m}^{-2} \text{ At}^{-1}$	Same
Remobilization				
Carbohydrate	$\text{g} [\text{CH}_2\text{O}] \text{ m}^{-2} \text{ At}^{-1}$	Non-structure $[\text{CH}_2\text{O}]$, S/D	$\text{g} [\text{CH}_2\text{O}] \text{ m}^{-2} \text{ At}^{-1}$	Wilson (1987b)
N exportation	$\text{g N m}^{-2} \text{ At}^{-1}$	Structure age, min N, S/D	$^{15}\text{D}^b$, N% of mass	Mae and Ohira (1982)
N recovery	$\text{g N m}^{-2} \text{ At}^{-1}$	Structure age, max N, S/D	^{15}D , N% of mass	Mae <i>et al.</i> (1983)
Priority				
Tiller age-cohort	None	Tiller age-cohort	None	Life table analysis data 1993
Structures	None	Type of structure	None	Tanaka <i>et al.</i> (1964)
Age class	None	Age of a structure	None	No data

(Continued)

Table 1—contd

<i>Process</i>	<i>Unit</i>	<i>Regulating variable</i>	<i>Unit</i>	<i>Data source</i>
Allocation				
Grains	$\text{g} [\text{CH}_2\text{O}]$ or $\text{N m}^{-2} \Delta t^{-1}$	$\text{S}^c, \text{D}_i^d, \text{P}_i^e$	$\text{g m}^{-2} \Delta t^{-1}$ $\text{g m}^{-2} \text{At}^{-1}$, none	Same sources as cited in Supply, Demand and Priority sections
Panicle branches	Same	$\text{S}, \text{D}_i, \text{P}_i$	Same	Same
Leaf blades	Same	$\text{S}, \text{D}_i, \text{P}_i$	Same	Same
Clums	Same	$\text{S}, \text{D}_i, \text{P}_i$	Same	Same
Leaf sheaths	Same	$\text{S}, \text{D}_i, \text{P}_i$	Same	Same
Roots	Same	$\text{S}, \text{D}_i, \text{P}_i$	Same	Same
Reserve	Same	$\text{S}, \text{D}_i, \text{P}_i$	Same	Same
Birth				
Tiller	$\text{Tillers m}^{-2}, \text{At}^{-1}$	$\text{S/D}, \text{N}^f$	None, N% of mass	Life table analysis data 1993
Grains	$\text{Grains tiller}^{-1}, \Delta t^{-1}$	$\text{S/D}, \text{Mass at PI}^g$	None, g plant ⁻¹	Destructive sampling 1992
Panicle branches	$\text{Branches m}^{-2} \text{At}^{-1}$	Nodes, N	$\text{Nodes maintiller}^{-1}$	Life table analysis data 1993
Leaf blades	$\text{Leaf blades m}^{-2} \Delta t^{-1}$	$\text{S/D}, \text{N}$	None, N% of mass	Same
Culms	$\text{Culms m}^{-2} \text{At}^{-1}$	$\text{S/D}, \text{N}$	Same	Same
Leaf sheaths	$\text{Leaf sheaths m}^{-2} \text{At}^{-1}$	$\text{S/D}, \text{N}$	Same	Same
Roots	$\text{Roots m}^{-2} \Delta t^{-1}$	$\text{S/D}, \text{N}$	Same	Same
Growth and aging				
Grains	g m^{-2}	Allocation, ϵ^h	g m^{-2} , none	Leaf tagging data 1992 Life table analysis data 1993
Panicle branches	Same	Same	Same	Same
Leaf blades	Same	Same	Same	Same
Culms	Same	Same	Same	Same
Leaf sheaths	Same	Same	Same	Same
Roots	Same	Same	Same	Same

Table 1—contd

Death				
Tiller	Tillers $\text{m}^{-2} \text{At}^{-1}$	S/D, N, Max age	None, N% of mass, °D	Life table analysis data 1993
Grains	Grains tiller $^{-1}$ At	S/D, N, Max age	Same	Panicle tagging data 1993
Panicle branches	Branches $\text{m}^{-2} \text{At}^{-1}$	S/D, N, Max age	Same	Same
Leaf blades	Leaf blades $\text{m}^{-2} \Delta t^{-1}$	S/D, N, Max age	Same	Life table analysis data 1993
Culms	Culms $\text{m}^{-2} \Delta t^{-1}$	S/D, N, Max age	Same	Same
Leaf sheaths	Leaf sheaths $\text{m}^{-2} \text{At}^{-1}$	S/D, N, Max age	Same	Same
Roots	Roots $\text{m}^{-2} \text{At}^{-1}$	S/D, N, Max age	Same	Same
Soil N balance				
Mineralization	$\text{g} [\text{NH}_4^+ - \text{N}] \text{m}^{-3} \text{At}^{-1}$	Organic matter, C/N ⁱ	g m^{-3} , none	Gilmour et al. (1985)
Nitification	$\text{g} [\text{NO}_3^- - \text{N}] \text{m}^{-3} \text{At}^{-1}$	NH_4^+	$\text{g} [\text{NH}_4^+ - \text{N}] \text{m}^{-3}$	Turner (1979)
Denitrification	$\text{g} [\text{NO}_3^- - \text{N}] \text{m}^{-3} \text{At}^{-1}$	Nitrate	$\text{g} [\text{NO}_3^- - \text{N}] \text{m}^{-3}$	Reddy (1982)
Clay N fixation	$\text{g} [\text{NH}_4^+ - \text{N}] \text{m}^{-3} \text{At}^{-1}$	NH_4^+ , Soil fixed NH_4^+	$\text{g} [\text{NH}_4^+ - \text{N}] \text{m}^{-3}$	Chen et al. (1989)
Ammonia volatilization	$\text{g} [\text{NH}_4^+ - \text{N}] \text{m}^{-3} \Delta t^{-1}$	Kinds of fertilizer, pH, Application method	Non, non	Reddy (1982)
Fertilization	$\text{g} [\text{NH}_4^+ - \text{N}] \text{m}^{-3}$	Amount of fertilizer	None	Mikkelsen et al. (1978)
Nitrogen uptake	$\text{g N m}^{-3} \text{At}^{-1}$	Root surface areas	g N m^{-3}	
		NH_4^+ , N demand	$\text{m}^2 \text{g}^{-1} \text{root}$	
			$\text{g} [\text{NH}_4^+ - \text{N}] \text{m}^{-3}$, g N m^{-2}	Youngdahl et al. (1982)

^a Δt =simulation time step (40 degree-days > 10°C).

^bD=cumulative degree-days greater than 10°C from the structure initiation.

^cS=supply.

^dD_i=demand of structure i.

^eP_i=priority of structure i.

^fN=nitrogen content of a plant.

^gPI=panicle initiation.

^h ϵ =the proportion of mass or numbers moving into the next age-class each simulation step.

ⁱC/N=carbohydrate/nitrogen ratio in organic matter.

verify and validate RICEPSM, field experiments were conducted in 1992 and 1993 at the Texas A&M University System Agricultural Research and Extension Center at Beaumont, Texas. The 1992 and 1993 field experiments both used a completely randomized plot design. In 1992, the rice was drill-seeded on May 8 at a rate of 90 kg ha^{-1} with a 0.18 meter-row spacing. When rice seedlings reached the third to fourth leaf stage, plants were hand thinned to a uniform density of about 20 plants per meter-row. Nitrogen fertilizer (ammonium sulfate) was applied at a rate of 90 kg N ha^{-1} before planting, 45 kg N ha^{-1} before permanent flooding, and 45 kg N ha^{-1} at panicle differentiation. The herbicide Propanil ($3.92 \text{ kg Al ha}^{-1}$) and the insecticide Furadan ($0.56 \text{ kg Al ha}^{-1}$) were used to suppress weeds and rice water weevil on June 3 and June 25, respectively. In 1993, the rice was drill-seeded on March 27 at a rate of 180 kg ha^{-1} and hand thinned to a uniform density of about 20 plants per meter-row as 1992. Propanil ($3.92 \text{ kg Al ha}^{-1}$) and Furadan ($0.56 \text{ kg Al ha}^{-1}$) were used to suppress weeds and rice water weevil on May 18 and May 29, respectively.

Twelve and six plots each were reserved for destructive sampling in 1992 and 1993, respectively. Each plot had six rows by 6 m, and was divided into six subplots. Rice grown in the center four rows and center 0.5 m of a subplot was destructively sampled in 1992, while samples were taken from the center four rows and 0.33 m of a subplot in 1993. During both years, sampling frequency was twice a week prior to panicle differentiation and once a week thereafter. Rice plants were removed with the soil to a depth of 40 cm to collect all roots. Samples were washed and divided into four groups: (1) main tillers arising from seeds, (2) first two sub-tillers of a main tiller, (3) third and fourth sub-tillers of a main tiller, and (4) the remaining sub-tillers. Tillers in each group were separated into five structural categories: root, stem (culm and leaf sheath), leaf blade, panicle vegetative component (branches and rachis), and grain. Measurements for each tiller group included: (1) number of tillers, (2) nodes per tiller, (3) leaf area (measured using a model CI-251 leaf area meter, CID, Inc.), and (4) number of filled and unfilled grains per panicle. All samples were oven-dried at 75°C to a constant weight, and each structure category for each tiller group was weighed.

In addition, 20 leaves from each position (leaves arising from the same node of the culm) for each group were subsampled once a month, and the length, width, and area of each leaf was measured. Three to four hundred newly emerging leaves ($< 3 \text{ cm}$ long) were tagged on each of three dates corresponding to early tillering, panicle differentiation, and flag leaf emergence. Two to three times a week, 20 tagged leaves were randomly harvested from each tagging. Each leaf was measured for leaf area, oven-dried, and weighed. These data were used to derive an average leaf growth curve for each of the three leaf cohorts. About 300 plants were tagged upon emergence

of each panicle from its flag leaf sheath (the visible part of a panicle < 10 cm long). Two to three times a week, 20 tagged panicles were collected. The number of unfilled (includes partially filled) and filled spikelets (grain) were counted, oven-dried, and weighed. These data provided estimates of the number of spikelets per panicle, grain size, growth rate, and proportion of filled spikelets. The field experiments are described in detail by Wu (1996).

Model structure

Table 2 summarizes the major physiological processes and functions within RICEPSM. RICEPSM is comprised of subpopulations of tillers of different ages, with each tiller consisting of panicles, stems (culm plus leaf sheath), leaves, and roots, each characterized by numbers, biomass, and age structure. Tillers are categorized into 12 age-cohorts based on the time at which they are initiated. The mass for each structure type within each tiller age-cohort for each age class is comprised of structural and non-structural carbohydrate, and nitrogen.

Initiation, growth, and development of each structure (leaf, root, sheath, culm, grain) is based on a physiological or degree-day time scale which was calculated using the double-sine approximation method (Allen, 1976). A 10°C lower temperature threshold for rice growth and development was obtained from the literature (Yoshida, 1981; Liang, 1983). For each time step, plant carbohydrate and nitrogen balances are used in simulating aging, and tiller and structure specific initiation and senescence rates. The time step for the population processes is 40 degree-days ($^{\circ}\text{D}$) $> 10^{\circ}\text{C}$, except for photosynthesis and respiration which are simulated hourly. A 40°D time step coincides with a 2 to 3 day time interval during the summer months. The time step is sufficiently small to match the sampling interval for the most detailed aspects of the field experiments.

A distributed-maturation algorithm (Plant and Wilson, 1986) is used to simulate the dynamics of organ initiation, growth, aging, and senescence. This equation integrates the intrinsic variability in structural growth and aging, estimated from field data, based on the McKendrick equation (McKendrick, 1926; Von Foerster, 1959). Each plant structure type has l_k age classes (l_k is equal to the ratio of the k th structure's developmental duration divided by the length of a time step) and l_k differential equations specifying the change in mass or numbers each time step.

Light interception and photosynthesis

Light interception is simulated using a layered canopy submodel (Wilson *et al.*, 1987a,b). The amount of incident solar radiation intercepted by each layer of leaves with common age depends on its leaf area index (LAI_j) and is

TABLE 2

A Summary of Major Equations used in RICEPSM

Process	Equation	Descriptions
Light interception	$PAR_{j,i} = PAR_{0,i}(e^{-aLAI_{j,l}} - e^{-aLAI_l})$	$PAR_{j,i}$: PAR intercepted by the j th leaf layer at the i th hour of a day; $PAR_{0,i}$: the light intensity above the leaf canopy at the i th hour of a day; a : the light extinction coefficient
Photosynthesis rate	$P_{g,j,i} = 31.5657(1 - e^{-0.009296PAR_{j,i}})$	$P_{g,j,i}$: the potential gross photosynthesis rate ($\mu\text{mol CO}_2\text{m}^{-2}$ leaf area s^{-1}) minus photo-respiration, for the j th leaf layer, at the i th hour of a day, at the optimum temperature and leaf nitrogen content. $PAR_{j,l}$ (μ Einstein's $\text{m}^{-2}\text{s}^{-1}$) is the intensity of light intercepted by the j th leaf layer at the i th hour of a day
Temperature effect	$C_T = \begin{cases} -0.434 + 0.103^\circ\text{C} - 0.00184^\circ\text{C}^2 & 5 < ^\circ\text{C} < 51 \\ 0 & \text{Otherwise} \end{cases}$	$^\circ\text{C}$: mean temperature
Nitrogen effect	$C_N = \begin{cases} -0.197 + 0.521N_l - 0.0566N_l^2 & 0.4 < N_l < 8.8 \\ 0 & \text{Otherwise} \end{cases}$	N_l : leaf nitrogen content
Potential photosynthesis	$P_{g,i} = C_T * C_N * \sum_{j=1}^l (P_{g,j,i} * LAI_j) * 3600$	l : the number of leaf layers; LAZ : leaf area index
Respiration	$R_m = (r_r * m_r + r_s * m_s + r_c * m_c + r_l * m_l + r_p * m_p + r_g * m_g) * Q_{10}^{(T-20)/10}$	m_r, m_s, m_c, m_l, m_p and m_g : mass of root, leaf sheath, clum, leaf blade, panicle vegetative component, and grain, respectively; r_r, r_s, r_c, r_l, r_p and r_g : respiration coefficient for each structure
Nitrification	$Nitrification_rate = (\Delta t/25) * 0.03175[NH_4^+ - N]^{1/4.17}$	Δt : the length of a time step
Clay N fixation rate	$\Delta Fixed_NH_4^+ = C1 * [NH_4^+ - N]$	$C1$: coefficient

Table 2—contd

Clay N release rate	$\Delta Released_NH_4^+ = C2 * ([Fixed_NH_4^+ - N] - 148)$	C2: coefficient
Plant uptake	$Uptake_i = 0.503 * [NH_4^+ - N_i] / (1.35 + [NH_4^+ - N_i] * Root_area_i)$	Root-area _i : the root surface areas in the ith soil layer
Root distribution	$P_x = \frac{\lambda^{nodes} * (x - \theta)^{nodes-1} * e^{-\lambda(x-\theta)}}{\Gamma(nodes)}$	nodes: the number of maintiller nodes, θ : the planting depth (cm); λ : a scale parameter; $\Gamma(nodes)$: a gamma function
Total carbohydrate and nitrogen demand	$DC_total = \sum_{j=1}^{12} DC_tiller_j$	DC_tiller_j : demand of the ith tiller cohort
Demand by the ith cohort	$DC_tiller_j = \sum_{k=1}^n \sum_{i=1}^{l_k} DC_m_{j,k,i}$	$DC_m_{j,k,i}$: the demand for carbohydrate by the ith age-class of the kth structure type, within the jth tiller age-cohort; l_k : the maximum number of age classes for the kth structure
Panicle growth rate	$m_p = m_{p,max} \left(\frac{0.9910}{1 + e^{16.168 - 0.0397 * Age_i}} \right)$	$m_{p,max}$: the maxim panicle vegetative mass; Age_i : the degree days from differentiation
N recovery	$Impt_N_i + (Max_N - Curt_N_i) * Mass_i * e^{-a * Age_i}$	Max_N : maximum potential nitrogen content; $Curt_N_i$: current nitrogen content; $Mass_i$ (g m ⁻²): mass of the ith age class of a structure; Age_i : the physiological age of the ith age class; a : coefficient
N export	$Expt_N_i = (Curt_N_i - Min_N) * Mass_i * (1 - e^{-b * Age_i})$	Min_N : the minimum nitrogen content; b : coefficient

Table 2—contd

Process	Equation	Descriptions
Priority	$P_i = \frac{m_{i,s}/m_{i,ns}}{\max(m_{i,s}/m_{i,ns})}$	$m_{i,s}$ and $m_{i,ns}$: either the final mass or the rate of mass increase of the <i>i</i> th category growing under physiological stress and under non-stressed conditions, respectively
N effect	$N_coef = \begin{cases} 1 & \text{if } N \geq N_c \\ \left(\frac{N}{N_c}\right) & \text{Otherwise} \end{cases}$	N and N_c : the current and critical nitrogen content
S/D effect	$SD_coef = \begin{cases} 1 & \text{if } \min(SD_n, SD_c) > 1 \\ (\min(SD_n, SD_c)) & \text{Otherwise} \end{cases}$	SD_n and SD_c : the potential nitrogen and carbohydrate supply/demand ratio
Node production rate	$\Delta Node = \Delta Node_{max} * N_coef * SD_coef$	$\Delta Node_{max}$: the maximum node production rate
Growth	$Growth_i \leq \begin{cases} Demand_i & \text{if } Supply_i \geq Demand_i \\ Supply_i * \frac{Demand_i * P_i}{\sum_{i=1}^n (Demand_i * P_i)} & \text{Otherwise} \end{cases}$	$Demand_i$: the demand of the <i>i</i> th category; $Supply_i$: the metabolite supply for the <i>i</i> th category

calculated based on a discretization of Beer's Law (Monsi and Saeki, 1953), where the layering of leaf age classes within the canopy was estimated from field data. The effect of photosynthetically active radiation on the potential photosynthetic rate was estimated using data from Tanaka *et al.* (1966), scaled to a maximum photosynthetic rate of $31.57 \mu \text{mol CO}_2 \text{ m}^{-2} \text{ leaf area s}^{-1}$ (Bouhache and Bayer, 1993; Sinclair and Horie, 1989). The data were scaled to correct for a consistent bias of earlier rice photosynthesis studies (Yoshida, 1981). Photosynthetic efficiency is a function of temperature (Huang *et al.*, 1990) and leaf nitrogen content (N_l) (Dingkuhn *et al.*, 1990). However, if the demand for carbohydrate is less than the potential supply, the gross photosynthetic rate is equal to the demand rate, reflecting carbohydrate supply driven photosynthesis feedback inhibition.

Respiration

Respiration in RICEPSM is separated into maintenance and growth respiration. Maintenance respiration is a temperature and mass dependent process with $Q_{10} = 2$ (Liang *et al.*, 1986; Tanaka *et al.*, 1966). Different structures have different physiological activities and therefore different respiration rates (Hesketh *et al.*, 1971; Penning de Vries and van Laar, 1982). At 20°C, leaves require 1.71% of their carbohydrate mass for daily maintenance respiration (Okano *et al.*, 1984). Stems, roots and reproductive structures are assumed to have 75, 25 (Iwaki, 1975, as cited by Graf *et al.*, 1990b), and 50% (Graf *et al.*, 1990b) of the per mass unit basis respiration rate of leaves, respectively. Growth respiration is treated as a function of photosynthetic activity (McCree, 1974). The coefficient for growth respiration is 0.27 (Yoshida, 1981). This means that 1 g of photosynthate not consumed by maintenance respiration produces 0.73 g dry mass.

Soil nitrogen transformation

The soil was divided into 10 layers, each 10 cm in thickness. The soil nitrogen balance for both NH_4^+-N and NO_3^--N was estimated each time step for each layer, taking into account mineralization, nitrification, denitrification, clay fixation, volatilization, and plant uptake (Standford *et al.*, 1975; Gilmour, 1984; Gilmour *et al.*, 1985; Jayaweera and Mikkelsen, 1990). All soil layers are assumed to be reduced except for the top 1 cm of the first soil layer, which is oxidized. Nitrogen transformation and uptake is calculated for each soil layer.

The method developed by Gilmour *et al.* (1985) is used to estimate the net rate of mineralization and immobilization. The relation between nitrification rate and the concentration of NH_4^+-N was estimated from data in Turner (1979). The fixation of ammonium N by clay and organic matter is assumed to be a reversible process between fixed NH_4^+-N and free NH_4^+-N in the

soil (Datta *et al.*, 1987; Keerthisinghe *et al.*, 1984; Schnier *et al.*, 1987). The $\text{NH}_4^+\text{-N}$ fixation rate is assumed to be a function of free $\text{NH}_4^+\text{-N}$ concentration, while the $\text{NH}_4^+\text{-N}$ release rate is a function of the fixed $\text{NH}_4^+\text{-N}$ concentration.

Plant nitrogen uptake

Nitrogen uptake from the *i*th soil layer by a growing root system is described by the Michaelis–Menten equation (Youngdahl *et al.*, 1982), and is a function of nitrogen concentration and root surface areas in the *i*th soil layer. The production of new roots at a particular depth during a time step is estimated using a three parameter Gamma distribution, as a function of node production and planting depth. The kinetics of $\text{NO}_3^-\text{-N}$ uptake is similar to that of $\text{NH}_4^+\text{-N}$. However, since the presence of $\text{NH}_4^+\text{-N}$ inhibits the uptake of $\text{NO}_3^-\text{-N}$ (Youngdahl *et al.*, 1982), $\text{NO}_3^-\text{-N}$ was assumed to be taken up by plants only when the uptake of $\text{NH}_4^+\text{-N}$ could not satisfy the demand by the plants.

Potential carbohydrate and nitrogen demand

The potential growth rates for leaves, root, culm, leaf sheath, and grain were estimated from the field experiments. Since main tiller vegetative growth is normally not source limited, the maximum potential mass of each structure type for all tiller age-cohorts is assumed to be the average observed maximum mass of the same structure type for the main tiller (age-cohort 1), except for grains, which are produced during a period of carbohydrate and nitrogen supply stress. The maximum mass for individual grain was estimated as the mean mass of the largest five grains observed from a sample of 100 grains, with the relative growth rate of grain estimated from destructively sampling panicles throughout their development. The maximum mass for the panicle vegetative component and for spikelets were estimated from the panicle tagging data, while published data (Nagai, 1959) were used to estimate panicle vegetative growth as a function of degree days from panicle differentiation.

Nitrogen dynamics in rice is complex and some simplifying assumptions were made: (1) each structure type has a maximum and minimum potential nitrogen content, (2) newly formed mass has the ability to reach its structure's maximum potential nitrogen content, and (3) the nitrogen demand for newly formed mass is proportional to the growth of each structure, suggesting an optimal nitrogen to carbohydrate ratio in plant tissues (Dingkuhn *et al.*, 1990).

Remobilization

If the potential carbohydrate supply is less than the corresponding demand, a maximum of 30% of non-structural carbohydrate is assumed to be

remobilized each 40°D time step. Remobilization of carbohydrates is processed using the same approach as described in the *Metabolite allocation priority* section. Previous research has shown that nitrogen is exported from mature leaves and redistributed to developing organs (Mae and Ohira, 1982; Makino *et al.*, 1984). However, nitrogen also continues to be imported into mature leaves during the period of net nitrogen export (Mae *et al.*, 1983). If the potential supply of nitrogen is greater than the demand required to produce new tissues, referred to as growth demand, a structure can recover nitrogen if its nitrogen content is less than its maximum potential content. The maximum amount of nitrogen imported into the *i*th age-class of a structure type is assumed to be a function of a structures mass and age, and the difference between its maximum potential nitrogen content and its current nitrogen content. If the potential supply is less than the growth demand, remobilizable nitrogen can be exported from structures having a lower allocation priority to satisfy or partially satisfy growth demand of higher priority structures. The maximum amount of nitrogen exported from a structure is also assumed to be a function of a structures mass and age, and the difference between its current nitrogen content and its minimum potential nitrogen content.

Metabolite allocation priority

RICEPSM uses a tiered metabolite allocation scheme: (1) metabolite allocation among tiller age-cohorts, (2) allocation among structures within a tiller age-cohort, and (3) allocation among age-classes within a structure type within a tiller cohort. At each level, the allocation priorities were estimated from the field experiments and from published data (Tanaka *et al.*, 1964; IRRI, 1986), based on the method of Wilson and coworkers (Wilson and Gutierrez, 1980; Wilson and Waite, 1982; Wilson *et al.*, 1987a,b; Pickett *et al.*, 1989).

Organ initiation

Rice has the property of synchronous initiation of a leaf blade, a leaf sheath, a culm, a tiller, and associated roots (Yoshida, 1981; Liang *et al.*, 1986). The maximum node production rate was estimated from the field data, by regressing the first four node estimates against cumulative degree days. When the *n*th node is initiated, the *n*th leaf blade, (*n*−1) leaf sheath, (*n*−2) culm, and (*n*−3)th tiller and roots are born. However, when rice plants have fewer than four nodes, the main tiller roots may not follow this rule (Liang *et al.*, 1986). When the last node is initiated, the panicle vegetative component and its grain are initiated. The number of spikelet positions per tiller was estimated as a function of the tiller's mass and rice population density (main tillers plus sub-tillers) at the time of panicle differentiation.

Analyses of published data (Liang *et al.*, 1986) suggests that the node production rate is a function of the ratio of the nitrogen content (N) in the plant and a critical nitrogen content (N_c) below which the rate decreases. The rate of node production is also affected by carbohydrate and nitrogen metabolic stress. With only limited information available for a mechanistic interpretation of carbohydrate and nitrogen supply/demand mediated node production, an assumption was made that node production is primarily governed by the rate limiting stress factor (either carbohydrate or nitrogen).

Organ growth

For each time step, each structure that had the potential to grow received some energy, with the amount received being a function of a structure's potential growth rate, its priority for metabolites, and the availability of carbohydrate and nitrogen to meet demands for growth.

Organ senescence

Nitrogen deficiency hastens senescence (Dingkuhn *et al.*, 1990). All structures within an age class senesce if the nitrogen content is lower than its minimum critical nitrogen content (van Keulen, 1978). Nitrogen deficiency induced tiller senescence was assumed to only occur prior to a tiller initiating panicle development. The senescence rate of a tiller age-cohort was assumed to be a function of its age and the rate limiting stress factor (either nitrogen or carbohydrate). As tillers senesce, the associated non-structural carbohydrates within the culm, leaf sheath, leaf blade, and root tissues are remobilized. The rates for spikelet degeneration and grain abortion are a function of carbohydrate and nitrogen stress occurring during the period from panicle differentiation to spikelet fertilization.

Meteorological variables

Daily maximum and minimum air temperatures, and solar radiation were recorded at the Texas A&M University System Agricultural Research and Extension Center at Beaumont. A subroutine obtained from Wilson *et al.* (1987b) was used to estimate hourly temperature and solar radiation from daily data.

Model parameterization, verification, and validation

The goodness of fit of the simulation model to observed data was evaluated using the coefficient of multiple determination (R^2), which measures the proportion of variability for single and multiple data types that was explained by the simulation model. Goodness of fit was evaluated across

sampling dates for 13 data types obtained from the 1992 and 1993 destructive sampling experiments: total dry mass, number of tillers, number of nodes per main tiller, and mass of root, stem, leaf blade, panicle vegetative component, and grain, for the main tiller and collectively for the sub-tillers (eqn (1)):

$$R^2 = 1 - \frac{\sum_j SSE_j / S_j^2}{\sum_j SSTO_j / S_j^2} \quad (1)$$

where $SSTO_j$ is the observed variation for the j th data type corrected for the mean, SSE_j is the amount of variability for the j th data type not explained by the model, and S_j^2 is the variance of the j th data type.

The 1992 and 1993 destructive sampling data sets were used to verify and validate the model, respectively. A critical value ($R_c^2 = 0.85$) was used to test overall goodness of fit. When R^2 was greater than the R_c^2 , the model was considered verified with respect to its fit to a data set, if compared with a data set used to parameterize the model; or validated, if compared with an independent data set. After the model was verified or validated against a data set, the previously unused data set was used to evaluate the goodness of fit. If the model failed to adequately fit a data set, the parameterization and analysis cycle was repeated until the model was verified or validated against both data sets. Once a data set has been used for parameterization or verification, it could be used to reparameterize the model but was no longer used for validation.

RESULTS

Model parameterization, verification, and validation

Table 3 summarized the parameters and functions estimated from the field experiments and used to parameterize the simulation model. Table 4 summarized the accuracy of the initially parameterized model at simulating the seasonal dynamics of the 13 data types. The fit of the simulation model to the 1992 destructive data set was separated into early-, mid-, and late-season for the growth and development of leaf, stem, and root mass, numbers of nodes per tiller and number of tillers. These three periods roughly corresponded to the time intervals from planting to panicle differentiation, from panicle differentiation to heading, and from heading to the final sample. For both the vegetative component of the panicle and its grain, early, mid, and

TABLE 3
Parameters and Functions Estimated from the Field Experiments

<i>Parameters</i>	<i>Value or function</i>	<i>Unit</i>
$ANode_{max}$	0.6280	Node At-'
ε^a	0.1096	None
$m_{l, max}^b$	0.2540	g leaf ⁻¹
$m_{c, max}$	0.3108	g node ⁻¹
$m_{s, max}$	0.3789	g node-'
$m_{r, max}$	0.1012	g node-'
$m_{p, max}$	0.1200	g panicle-'
$m_{g, max}$	0.0321	g grain-'
Number of grains	$232.52 + 59.11m_l - 0.413Density^c$	grains panicle-'
Specific leaf area	$-1.7248e-11D^3 + 6.2908e-8D^2 - 7.5313e-5D^d + 0.04987$	m ² g ⁻¹

^a ε is the probability of aging 2 age classes each time step for leaf, stem, root, vegetative panicle and grain.

^b $m_{l, max}$ is mass for the largest leaf of main tiller.

^c m_l and *density* are the tiller mass (g tiller-'), and tiller density (tillers m⁻²) at panicle differentiation.

^dD is degree-days (> 10°C) from planting.

TABLE 4
The Relative Departure of Simulated from Observed Data for the 1992 Verification Data Set^a

<i>Data type</i>	<i>Maintiller growth stage</i>			<i>Subtiller growth stage</i>		
	<i>Early-</i>	<i>Mid-</i>	<i>Late-</i>	<i>Early-</i>	<i>Mid-</i>	<i>Late-</i>
Note number	--	0	0			
Tiller number				++	+/-	--
Leaf mass	0	+	++	++	++	+
Stem mass	0	-	0	++	++	+
Root mass	0	-	0	++	++	+
P. vegetative mass	-	--	-	+	--	--
Grain mass	0	+	++	+	+	-
Total mass	+	+	++			

^a0 the model closely simulated the observed data, + and ++ model overestimated data type by 5–10% and >10%, respectively, - and -- underestimated by 5–10% and > 10%, respectively.

late roughly corresponded to three successive 400°D time interval starting from panicle differentiation. A 0 in Table 4 indicates that the model closely simulated the observed data. A + or - indicates that the model overestimated or underestimated the data type by 5 to 10%. A ++ or -- indicates that the model consistently departed by greater than 10% from the observed data during the indicated time period.

The model failed to pass the verification step following initial parameterization. An analysis of Table 4 indicated that the model accurately simulated number of nodes and main tiller mass during the early- and mid-season periods. However, subtiller mass was overestimated, while main tiller root mass and panicle vegetative mass were underestimated. As assumption had been made that the maximum potential mass of a structure was the same for all structures of a type that were initialized at the same time, for all tiller cohorts. An analysis of the 1992 leaf mass data showed that the maximum mass for the first 3 to 4 leaves decreased with each successive tiller cohort. An assumption had also been made that this decrease was largely due to leaves on young sub tillers having a lower potential for growth. An error was also identified with the procedure used to initiate panicle differentiation. When the number of nodes per main tiller reached the average node at which panicle differentiation occurred (11 for Gulfmont), all tillers had been triggered to initiate panicle development. This approximation was incorrect since 10 to 14 days are required to complete panicle differentiation for all the tillers in a field (Liang *et al.*, 1986; Yoshida, 1981). Analysis of the node production data showed that the number of nodes per main tiller in each sample followed a normal distribution with a standard deviation of 0.498. In the reparameterized model, for each time step, the proportion of main tiller and sub tillers reaching panicle differentiation was estimated as the probability of a main tiller having ≥ 11 nodes.

This change resulted in improvement to the simulated output, but the model again failed the verification test. The primary cause for the lack of fit of the simulated data to the observed data was traced to the function which controlled tiller initiation and senescence, and the functions which controlled spikelet production and abortion. The initially parameterized model assumed that tiller production and survival were at a maximal rate when the carbohydrate S/D ratio was ≥ 1.0 . However, the destructive sampling data indicated that the rate of tiller production and the tiller survival rate both began to decrease prior to the time when either carbohydrate or nitrogen stress were simulated to occur. This may suggest that localized source-sink imbalances may reduce tiller initiation and increase mortality when whole plant estimates of carbohydrate production appear sufficient to meet total plant demands. Or, it may indicate that the plant is able to detect changing carbohydrate levels as carbohydrate stress is approached, possibly by detecting the gradual release of photosynthesis from feedback inhibition as carbohydrate demand rapidly approaches carbohydrate supply. The fit of the simulated model was improved by changing the potential carbohydrate S/D ratio at which maximum tiller initiation and survival occurs from 1.0 to 1.1. The lack of fit of the spikelet data was due to having assumed that spikelets initiated development at the time of panicle differentiation, which coincides

with emergence of the third leaf from the flag leaf. Spikelet production on a differentiating panicle actually occurs at the time of the emergence of the 2nd leaf from the flag leaf (Yoshida, 1981). This correction only partially accounted for the discrepancy between observed and simulated spikelet production and survival. The simulated spikelet numbers overestimated the observed data and underestimated spikelet mortality, particularly during the period of spikelet production and grain filling. This appeared largely due to the lack of inclusion of the direct impact of high temperatures on spikelet abortion as had been documented by Liang *et al.* (1986). As a result, eqn (2) was added to integrate the impact of daily temperatures on spikelet abortion:

$$Abortion = \begin{cases} 0.00025(T - 27)^2 & T \geq 27 \\ 0 & 24 < T < 27 \\ 0.0025(24 - T)^2 & T \leq 24 \end{cases} \quad (2)$$

where *Abortion* is the proportion of spikelets aborted per day, and T is a daily mean temperature (°C) during the time from spikelet differentiation to 10 days after flowering.

Model output was significantly improved with the criteria for model verification having been met (Table 5). The verified model was then used to simulate rice growth and development using the 1993 agronomic and weather data, and the simulated output compared with the 1993 data set. The model met the validation criteria without further modification (Table 5). Although the model was verified with the 1992 data set and validated with the 1993 data set, comparison of the simulated results to both the 1992 and 1993 data sets showed that simulated leaf and stem mass were greater than the observed mass for both years following the initiation of grain filling. These discrepancies suggest that the model either overestimated leaf and stem initiation, overestimated the growth rate of individual leaves and stem segments, underestimated remobilization of mass from these structures to other structures, or overestimated leaf and stem longevity. Comparison of the number of simulated nodes per meter square (cumulative leaf or stem initiation) with observed number of nodes in 1992, for both the main tillers and sub-tillers, indicated that stem and leaf initiation were simulated accurately ($r^2=0.92$). Similarly, comparison of simulated and observed growth rates for late season produced leaves indicated close fit to the 1992 leaf data ($r^2=0.96$). Remobilization of nonstructural carbohydrate and nitrogen were each estimated from data obtained from the literature (Andrews, 1990; Schnier *et al.*, 1990). As a result, their accuracy can not be directly evaluated. However, the close fit of the simulated and observed early- and mid-season leaf mass data suggests a lack of discrepancies comparing the literature derived estimates with the estimates derived from the 1992 and 1993 experiments.

TABLE 5
*R*² Values for Overall Model Fit and for Each Data Type for the 1992 and 1993 Data Sets

<i>Simulation</i>	<i>Total</i>		<i>Tiller</i>		<i>Main tiller mass (g m⁻²)</i>					<i>Subtiller mass (g m⁻²)</i>				
	<i>Overall</i>	<i>Mass</i>	<i>m²</i>	<i>Node^a</i>	<i>Panicle^b</i>	<i>Grain</i>	<i>Leaf</i>	<i>Stem</i>	<i>Root</i>	<i>Panicle</i>	<i>Grain</i>	<i>Leaf</i>	<i>Stem</i>	<i>Root</i>
Verification	0.69	0.82	0.60	0.97	0.69	0.68	0.76	0.89	0.69	0.00	0.81	0.56	0.74	0.40
Verification"	0.77	0.88	0.80	0.97	0.76	0.74	0.76	0.89	0.69	0.42	0.81	0.68	0.80	0.57
Verification ^d	0.83	0.90	0.88	0.98	0.79	0.83	0.81	0.88	0.80	0.64	0.81	0.73	0.88	0.73
Verification'	0.88	0.94	0.94	0.98	0.79	0.88	0.84	0.88	0.85	0.70	0.93	0.86	0.89	0.81
Validation 1993	0.87	0.97	0.84	0.99	0.86	0.92	0.92	0.91	0.96	0.64	0.95	0.75	0.87	0.65
Reverification 1992 ^f	0.92	0.97	0.96	0.98	0.84	0.92	0.92	0.92	0.84	0.90	0.96	0.91	0.88	0.86
Reverification 1993'	0.89	0.99	0.84	0.99	0.87	0.92	0.95	0.96	0.95	0.83	0.94	0.82	0.90	0.77

^aNumber of nodes per main tiller.
^bPanicle vegetative component.
"Addition of tiller cohort leaf potential size function, and distributed panicle differentiation node.
^dChange to tiller survival function, correction to spikelet initiation function.
'Addition of temperature spikelet abortion function.
^fCorrection to leaf duration estimate, addition of metabolic stress main tiller leaf sheath death function.

The lack of discrepancy between the simulated and estimated values with these components, suggests an error with the estimated leaf longevity. The original analysis of the 1993 life table data showed that leaf longevity was a function of nodal position. In addition, published data showed that leaf longevity was also a function of leaf nitrogen concentration (van Keulen, 1978; Tanaka *et al.*, 1964). Reanalysis of the 1993 life table data showed that the maximum leaf age at senescence for the last four leaves on each main tiller and subtiller (960°D) had inadvertently been used for the mean leaf longevity (880°D). Similarly, reanalysis of the destructive sampling data suggested that the stem discrepancy was due to the observed main tiller and subtiller stem mass decreasing more rapidly than the simulated mass. The 1992 and 1993 destructive sampling data showed that stem mass from the final sample ranged from 63 to 100% of the maximum stem mass depending on the tiller cohort, with the main tiller stem mass decreasing to the greatest degree followed in order by the successive tiller cohorts. These data imply that the main tiller stem had a relatively greater amount of mass remobilized to grain, and probably greater leaf sheath senescence. The greater reduction in main tiller stem mass was probably due to its greater sink size (number of spikelets per panicle). Although RICEPSM calculates sink size for each tiller age-cohort, it does not maintain separate metabolic pools for each tiller cohort. To capture the differential remobilization contrasting tiller cohorts, each time step that the potential carbohydrate S/D ratio was less than one, 3% of leaf sheath mass was removed from all leaf sheath age classes for the main tiller cohort, reflecting an increase in sheath senescence. The reparameterized model was then reverified against both the 1992 and 1993 data sets (Table 4).

Simulated vs observed data

The verified and validated rice model simulated reasonably well the node production rates comparing the two years ($r^2 = 0.98$, $n = 8$, 1992; $r^2 = 0.99$, $n = 13$, 1993). Before panicle differentiation, a node was produced about every 70 to 80°D ; afterwards every 100 to 140°D . The R^2 for the goodness of fit for number of nodes per main tiller was 0.97 and 0.99 for the 1992 and 1993 data, respectively. Accuracy in simulating tiller node production is critical to model performance since initiation of each structure type and each subtiller, and their subsequent growth are related to the initiation of the associated node. The lower rate of early node production during 1992 (on a degree-day time scale) was largely a result of increased temperatures due to the later planting date during that year, resulting in higher respiration rates and lower metabolic efficiency.

The number of tillers increased rapidly until a maximum number was reached at 930 and 750°D from planting, in 1992 and 1993, respectively (Fig. 1).

Fig. 1. Observed and simulated number of tillers (tillers m^{-2}) for the 1992 and 1993 experiments.

Analysis of the simulated seasonal carbohydrate supply/demand patterns suggests that the difference in tillering was due to transitory carbohydrate stress occurring just prior to the time of tiller initiation during 1992 (Fig. 2(A)), resulting from higher temperatures and elevated respiration rates experienced at that stage of crop growth. While tiller initiation appeared to be largely controlled by carbohydrate stress, the mid-season pattern of tiller senescence appeared to be caused by nitrogen stress (Fig. 2(B)). Although the simulated number of tillers in the late season was slightly higher than the observed data for the 1993 season, the model captured the seasonal dynamics of tiller initiation and senescence ($r^2=0.84$).

The rice model generally accurately simulated mass for leaf, stem, root, panicle vegetative component, and grain (Fig. 3), for the main tiller and sub-tillers (data not shown). However, in 1992, leaf mass was overestimated and root mass underestimated during grain ripening. In contrast, in 1993, root mass was overestimated for sub-tillers during grain ripening. Panicle vegetative mass for main tillers and sub-tillers were the least well simulated. The relatively poor fit of the simulation model to the panicle vegetative mass in 1992 appears due to rice blast (*Pyricularia grisea* Saccardo) affecting about 30–50% of the rice plants during grain filling. Comparison of the ratios of simulated to observed grain mass showed a higher ratio in 1992 (1.05) than in 1993 (0.93). In contrast, the comparable ratios for the panicle vegetative mass were lower in 1992 (0.87) than in 1993 (1.08). These results, although not conclusive, suggest that the rice blast may have inhibited transport of carbohydrates to the developing grain during 1992, causing carbohydrate loading in the panicle vegetative mass 'upstream' to the sites of partial phloem blockage.

Fig. 2. (A) Simulated potential carbohydrate supply/demand S/D ratio, and (B) simulated potential nitrogen S/D ratio for the 1992 and 1993 experiments.

DISCUSSION

The statistically rigorous parameterization, verification, and validation procedure forced us to examine in great detail each of the assumptions embedded within the model. As such, it improved our understanding of rice plant population dynamics. This activity has also resulted in a physiologically based model which has considerably potential for use in addressing the impact of physical and abiotic stresses on rice growth, development, and yield. The model's age-structure proved necessary for accurately capturing the distributed growth of the vegetative and reproductive structures. It also enabled us to discriminate the differential response of each age class of each plant part to stress, and will enable us to link RICEPSM with herbivore, pathogen, nematode, and weed population models. From a conceptual point of view, this approach can be used to study the dynamics of a range of cropping system.

The physiological detail imbedded within RICEPSM departs to the greatest degree from previously published rice simulation models in its tiller

Fig. 3. Observed and simulated dry mass accumulation of panicle vegetative component, grain, leaf, leaf sheath, culm, root, and total dry mass for the 1992 and 1993 experiments.

cohort and plant organ age structure, and its metabolite partitioning structure. Only the model by Graf *et al.* (1990a,b) had previously incorporated an age-structure that integrates variability in aging. Possibly the greatest distinction between our model and previously developed rice models is the inclusion of a statistically rigorous model parameterization, verification, and validation process. In most cases, authors of rice simulation models have concluded that their models were statistically validated based on the graphical fit of selected output to a data set from another year or location (McMennamy and O'Toole, 1983; Graf *et al.*, 1990b; Miller *et al.*, 1993), from data sets used to parameterize the model (Zhang and Chen, 1990), or by referencing obscure and often difficult to obtain proceedings articles. Although graphical comparison is the most straightforward and possibly the most commonly used method, the perceived level of deviation of simulated values from observed data depends on the scale chosen for presentation. For example, Miller *et al.* (1993) graphically compared simulated total mass, leaf, stem and grain mass with observed data, with the resultant fit appearing to

be quite good. However, r^2 values estimated from data in Miller *et al.* (1993) were 0.76 ($n=6$), 0.30 ($n=6$), 0.73 ($n=6$), and 0.93 ($n=3$), for above ground mass, leaf, stem, and grain mass, respectively; while R^2 across the four data types was 0.63.

Salam *et al.* (1994) used the r^2 value of the linear regression between the simulated and observed mass to evaluate their model. This method gives the correct result only when the Y intercept of the regression line is zero, and when the slope of the regression is 1.0. Graf *et al.* (1991) proposed two statistics, a standardized bias $R = \sum_{i=1}^n (y_i - x_i) / \sum_{i=1}^n x_i$, and a standardized mean square error $V = \sum_{i=1}^n (y_i - x_i)^2 / \sum_{i=1}^n x_i^2$. The authors incorrectly concluded that

“ R quantifies the model’s ability to reproduce the observed growth pattern”, and that V “reveals the model’s tendency to generally over- or under-estimate field observations”. The statistic R is flawed since negative deviations compensate for positive deviations. The statistic V only measures the total square relative deviation which does not indicate whether the model over- or under-estimates the observed data.

Willers *et al.* (1995) presented statistical methodology based on the generalized multiplicative interaction model (Milliken and Johnson, 1989) that could be used to test the fit of simulation models to a single response variable having a two-way unreplicated treatment structure. The generalized multiplicative interaction model is most appropriately used when an unreplicated two-factor analysis is biased due to a significant first-order interaction term. Because the first order interaction is used as the error term (fixed effect model) for such an analysis, it overestimates the true error when the interaction is significant, resulting in the significance of the main affects being underestimated (Zar, 1984).

The generalized multiplicative interaction model would have application to this research were the focus to have been on the difference between simulated and observed data for a single response variable, across two independent variables. However, the application of such an approach to each of the 13 response variables for each time that samples were taken, would have been analogous to conducting repeated t-tests, which would have resulted in major inflation of the α error rate. The resulting effect would be to conclude that a greater number of significant difference was present than was the case, resulting in an error opposite in direction to that which can occur when conducting non-replicated factorial analyses.

The verification-validation approach used in this paper has the advantage of enabling the individual and collective fit of multiple response variables to be examined. Furthermore, by analyzing the temporal ‘fit’ of the model, as

contrasted with a single point in time analysis as presented by Willers *et al.* (1995), it can be argued that the robustness of the simulation model can be better evaluated.

The value of RICEPSM to the scientific community will in part depend on how well this model performs across a range of plant types, physical and biotic stress levels, and geographical locations. The 1992 and 1993 experiments were planted May 8 and March 27, to insure that the temperatures experienced during vegetative and reproductive growth were quite different contrasting the two growing seasons. The mean temperature during the first month following planting was much warmer in 1992 ($\bar{x}=23.8^{\circ}\text{C}$) than in 1993 ($\bar{x}=18.0^{\circ}\text{C}$). In contrast, the mean temperature from heading to harvest was much lower in 1992 ($\bar{x}=25.8^{\circ}\text{C}$) than in 1993 ($\bar{x}=28.7^{\circ}\text{C}$). The excellent fit to both data sets suggests that the model captures the general effect of temperature on rice tiller population growth and development. Wilson *et al.* (1996) used RICEPSM to compare the yield response of 15 diverse rice types differing in the number of tillers produced, the node at which the panicle was initiated, the number of florets produced per panicle, and the average mass of each grain on the mature panicle, for each of two growing seasons (1994 and 1995). The yield of these lines varied from 492 to 1161 g m⁻² in 1994 and 227 to 706 g m⁻² in 1995, with harvest varying from 106 to 149 days after planting in 1994 and 113 to 158 days in 1995, respectively. Grain yield for the very early and very late maturing recombinant lines was very similar in 1994 and 1995. In contrast, the intermediate maturing lines suffered extreme reductions in grain yield in 1995 contrasted with 1994. Simulation analyses by Wilson *et al.* (1996) strongly suggested that the reductions in yields for the mid-season maturing lines was largely due to carbohydrate depletion caused by high night temperatures during the middle of the 1995 summer months. Subsequent analysis of total non-structural carbohydrate levels showed a 23% reduction during the 1995 grain filling period contrasted with values obtained in 1994 (Samonte and Wilson, unpubl. data). The ability of RICEPSM to capture the yield variability and carbohydrate depletion across recombinant inbred lines representing a wide range of growth patterns is very encouraging. In a third analysis, Wu and Wilson (1997) simulated the response of rice to rice water weevil injury, using four years of data obtained from the literature. Each year had up to three treatments representing an untreated control, a single, and two insecticide applications to suppress the rice water weevil. The treatments resulted in a range of rice water weevil population densities. In this analysis, an average of 95% of the variation in grain yield and above ground biomass was explained by the model, contrasting to only 58% of the variability explained by a multiple linear regression model. The general ability of RICEPSM to accurately capture rice's response to varietal differences, and

physical and biotic stresses is encouraging. A statistically rigorous parameterization, verification, and validation approach that is applicable for use in evaluating other crop simulation models is presented.

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REFERENCES

- Allen J. C., (1976) Modified sine wave method for calculating degree-days. *Environmental Entomology* **5**, 388–396.
- Andrews, D. L. (1990) Characterization of differentially expressed mRNA sequences in rice (*Oryza sativa* L.), cv. Lemont and correlation of their expression with total nonstructural carbohydrate content. Ph.D. dissertation, Texas A&M University, College Station, TX.
- Angus, J. F. and Zandstra, H. G. (1980) Climatic factors and the modeling of rice growth and yield. In *Proceedings of a Symposium on the Agrometeorology of the Rice Crop*, pp. 189–199. IRRI, Los Baños, The Philippines.
- Bouhache, M. and Bayer, D. E. (1993) Photosynthetic response of flooded rice (*Oryza sativa*) and three *Echinochloa* species to changes in environmental factors. *Weed Science* **41**, 611–614.
- Chen, C. C., Turner, F. T. and Dixon, J. B. (1989) Ammonium fixation by high-charge smectite in selected Texas Gulf Coast soils. *Soil Science Society of America Journal* **53**, 1035–1040.
- Costello, T. A., VanDecender, K. W. and Ferguson, J. A. (1988) The Arkansas rice model: preliminary structure. *ASAE Microfiche* No. 88-4062.
- Datta, S. K., Fillery, I. R. P., Obcemea, W. N. and Evangelista, R. C. (1987) Floodwater properties, nitrogen utilization, and nitrogen-15 balance in a calcareous lowland rice soil. *Soil Science Society of America Journal* **51**, 1355–1362.
- Dingkuhn, M., Schnier, H. F., De Datta, S. K., Dorffling, K., Javellana, C. and Pamplona, R. (1990) Nitrogen fertilization of direct-seeded flooded vs. transplanted rice: 11. Interactions among canopy properties. *Crop Science* **30**, 1284–1292.
- Gilmour, J. T. (1984) The effects of soil properties on nitrification and nitrification inhibition. *Soil Science Society of America Journal* **48**, 1262–1266.
- Gilmour, J. T., Clark, M. D. and Sigua, G. C. (1985) Estimating net nitrogen mineralization from carbon dioxide evolution. *Soil Science Society of America Journal* **49**, 1398–1402.

- Graf, B., Gutierrez, A. P., Rakotobe, O., Zahner, P. and Delucchi, V. (1990) A simulation model for the dynamics of rice growth and development. Part 11. The competition with weeds for nitrogen and light. *Agricultural Systems* **32**, 367–392.
- Graf, B., Rakotobe, O., Zahner, P., Delucchi, V. and Gutierrez, A. P. (1990) A simulation model for the dynamics of rice growth and development. Part I. The carbon balance. *Agricultural Systems* **32**, 341–365.
- Graf, B., Dingkuhn, M., Schnier, F. and Coronel, V. (1991) A simulation model for the dynamics of rice growth and development. 111. Validation of the model with high-yielding varieties. *Agricultural Systems* **36**, 329–349.
- Gutierrez, A. P. and Wang, Y. (1976) Applied population ecology: models for crop production and pest management. In *Proceeding of a Conference on Pest Management*, ed. C. Norton and C. S. Holling, pp. 352. Laxenberg, Austria.
- Hesketh, J. D., Baker, D. N. and Duncan, W. G. (1971) Simulation of growth and yield in cotton: respiration and the carbon balance. *Crop Science* **2**, 394–398.
- Huang, C. and Wang, T. D. (1986) Computer simulation of biomass production in rice community. *Acta Agronomica Sinica* **12**(1), 1–8.
- Huang, Y., Gao, L. Z. and Jin, Z. Q. (1990) A dynamic computer model for simulating photosynthetic production of rice canopies. *Chinese Agriculture Meteorology* **11**(1), 10–15.
- IRRI (1986) *Progress Report for 1985*. IRRI, Los Baños, The Philippines.
- Jayaweera, G. R. and Mikkelsen, D. S. (1990) Ammonia volatilization from flooded soil systems: a computer model. *Soil Science Society of America Journal* **54**, 1447–1468.
- Keerthisinghe, G., Mengel, K. and Datta, S. K. (1984) The release of non-exchangeable ammonium (^{15}N labelled) in wetland rice soils. *Soil Science Society of America Journal* **48**, 291–294.
- Liang, L. (1983) *Ecology of Rice*. Chinese Agriculture Press, Beijing.
- Liang, G. S., Muo, J. R. and Ran, C. F. (1986) Rice physiology and ecology. In *Rice Cultivation in China*, pp. 159–220. Chinese Academy of Agricultural Sciences. Chinese Agriculture Press, Beijing.
- Mae, T. and Ohira, K. (1982) Relation between leaf age and nitrogen incorporation in the leaf of the rice plant (*Oryza sativa* L.). *Plant and Cell Physiology* **23**, 1019–1024.
- Mae, T., Makino, A. and Ohira, K. (1983) Change in the amount of ribulose biphosphate carboxylase synthesized and degraded during the life span of rice leaf (*Oryza sativa* L.). *Plant and Cell Physiology* **24**, 1079–1086.
- Makino, A., Mae, T. and Ohira, K. (1984) Relation between nitrogen and ribulose-1, 5-biphosphate carboxylase in rice leaves from emergence through senescence. *Plant and Cell Physiology* **25**, 429–437.
- McCree, K. J. (1974) Equation for the rate of dark respiration of white clover and grain sorghum, as function of dry weight, photosynthetic rate, and temperature. *Crop Science* **14**, 509–514.
- McKendrick, A. G. (1926) The application of mathematics to medical problems. *Proceedings Edinburgh Mathematical Society* **44**, 98–130.
- McMennamy, J. A. and O'Toole, J. C. (1983) RICEMOD: a physiologically based rice growth and yield model. *ZRPS* **87**, 1–33.
- Miller, B. C., Foin, T. C. and Hill, J. E. (1993) CARICE: a rice model for scheduling and evaluating management actions. *Agronomy Journal* **85**, 938–947.

- Milliken, G. and Johnson, D. (1989) *Analysis of Messy Data. Vol. 2. Nonreplicated Experiments*. Van Nostrand Reinhold, New York.
- Monsi, M. and Saeki, T. (1953) Über den lichtfaktor in den pflanzengesellschaften und seine bedeutung für die stoffproduktion. *Journal of Botany, Japan* **14**, 22–52.
- Nagai, I. (1959) *Japonica Rice: Its Breeding and Culture*. Yokendo Ltd, Tokyo.
- Okano, K., Tatsumi, J., Yoneyama, T., Kono, Y. and Totsuka, T. (1984) Comparison of the rates of $^{15}\text{NO}_2$ and $^{13}\text{CO}_2$ absorbed through a leaf of rice plants. *Research Report from the National Institute for Environmental Studies, Japan* **66**, 59–68.
- Penning De Vries, F. W. T. and Van Laar, H. H. (1982) Simulation of growth processes and the model BACROS. In *Simulation of Plant Growth and Crop Production*, ed. F. W. T. Penning De Vries and H. H. Van Laar, pp. 114–135. Pudoc, Wageningen.
- Pickett, C. H., Wilson, L. T., Flaherty, D. L. and Gonzalez, D. (1989) Measuring the host preference of parasites: an aid in evaluating biotypes of *Anagrus Epos* [HYM: Mymaridae]. *Entomophaga* **34**, 551–558.
- Plant, R. E. and Wilson, L. T. (1986) Models for age structural populations with distributed maturation rates. *Journal of Mathematical Biology* **23**, 247–262.
- Reddy, K. R. (1982) Nitrogen cycling in a flooded-soil ecosystem planted to rice (*Oryza sativa* L.). *Plant and Soil* **67**, 209–220.
- Ritchie, J. T., Alcocilja, E. C., Singh, U. and Uehara, G. (1987) IBSNAT and the CERES-Rice model. In *Weather and Rice*, Proceedings of the International Workshop on the impact of weather parameters on growth and yield of rice, 7–10 April, 1986, pp. 270–279. IRRI, Los Baños, The Philippines.
- Salam, M. U., Street, P. R. and Jones, J. G. W. (1994) Potential production of Boro rice in the Haor region of Bangladesh: Part I. The simulation model, validation and sensitivity analysis. *Agricultural Systems* **46**, 257–278.
- Schnier, H. F., De Datta, S. K. and Mengel, K. (1987) Dynamics of ^{15}N -labelled ammonium sulfate in various inorganic and organic soil fractions of wetland rice soils. *Biological Fertilizer Soils* **4**, 171–177.
- Schnier, H. F., Dingkuhn, M., De Datta, S. K., Mengel, K. and Faronilo, J. E. (1990) Nitrogen fertilization of direct-seeded flooded vs. transplanted rice: I. Nitrogen uptake, photosynthesis, growth, and yield. *Crop Science* **30**, 1276–1284.
- Sinclair, T. R. and Horie, T. (1989) Leaf nitrogen, photosynthesis, and crop radiation use efficiency: a review. *Crop Science* **29**, 90–98.
- Singh, U. and Padilla, J. L. (1995) Simulating rice response to climate change. In *Climate change and Agriculture: Analysis of Potential International Impacts*, ed. G. A. Peterson, pp. 99–121. ASA Special Publication No. 59, Madison, WI.
- Standford, G., Dzienia, S. and Vanderpol, R. A. (1975) Effect of temperature on denitrification rate in soils. *Proceeding of Soil Science Society of America* **39**, 867–870.
- Tanaka, A., Kawana, K. and Yamaguchi, J. (1966) Photosynthesis, respiration, and plant type of the tropical rice plant. *Technical Bulletin* **7**, 1–46.
- Tanaka, A., Navasero, S. A., Garcia, C. V., Parao, F. T. and Ramirez, E. (1964) Growth habit of the rice plant in the tropics and its effect on nitrogen response. *Technical Bulletin* **3**, 3–77.
- Turner, F. T. (1979) Soil nitrification retardation by rice pesticides. *Soil Science Society of America Journal* **43**, 955–957.

- Van Keulen, H. V. (1978) Simulation of influence of climatic factors on rice production. In *Climatic Change and Food Production*, ed. K. Takahashi and M. M. Yoshino, pp. 345–358, University of Tokyo Press, Tokyo.
- Von Foerster, H. (1959) Some remarks on changing populations. In *The Kinetics of Cellular Proliferation*, ed. F. Stohlmán, pp. 382–407. Grune and Stratton, New York.
- Willers, J. L., Wagner, T. L., Sequira, R. A., Theseira, G. W. and Boykin, D. L. (1995) Analysis of deterministic simulation models using methods applicable to two-way treatment structures without replication. *Agronomy Journal* 87, 478–492.
- Wilson, L. T. and Gutierrez, A. P. (1980) Fruit predation submodel: *Heliothis* larvae feeding upon cotton fruiting structures. *Hilgardia* 48(2), 24–36.
- Wilson, L. T. and Waite, G. K. (1982) Feeding pattern of Australian *Heliothis* on cotton. *Environmental Entomology* 11, 297–230.
- Wilson, L. T., Gutierrez, A. P., Tennyson, R. and Zalom, F. G. (1987a) A physiological based model for processing tomatoes: crop and pest management. *Acta Horticulturae* 200, 125–132.
- Wilson, L. T., Plant, R. E., Kerby, T. A., Zelinski, L. and Goodell, P. B. (1987b). Transition from a strategic to a tactical crop and pest management model: use as an economic decision aid. In *1987 Proceedings Beltwide Cotton Production Research Conferences*, pp. 207–213. Dallas, TX.
- Wilson, L. T., Wu, G., Samonte, O. P. B. and Makela, M. E. (1996) Use of physiological modeling in quantifying the impact of weather on the 1995 late season yield decline. In *Proceedings 26th Rice Technical Working Group*, p. 134. Texas Agricultural Experiment Station, College Station, TX.
- Wu, G. (1996) Biological systems approach to analyzing population dynamics of rice and its response to major physical and biotic variables. Ph.D. dissertation, Texas A&M University, College Station, TX.
- Wu, G. W. and Wilson, L. T. (1997) Analysis of the growth and yield response of rice to rice water weevil injury. *Environmental Entomology* (in press).
- Yoshida, S. (1981) *Fundamentals of Rice Crop Science*. IRRI, Los Baños.
- Youngdahl, L. J., Pacheco, R., Street, J. J. and Vlek, P. L. G. (1982) The kinetics of ammonium and nitrate uptake by young rice plants. *Plant and Soil* 69, 225–232.
- Zar, J. H. (1984) *Biostatistical Analysis*. Prentice-Hall, Englewood Cliffs, NJ.
- Zhang, J. and Chen, C. G. (1990) Simulation of the dynamics of growth process and yield of rice population. *Acta Ecologica Sinica* 4, 311–316.