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A Functional Analysis of Pedotransfer Functions Developed for Sri Lankan soils: Applicability for Process-Based Crop Models

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Received: 14 January 2020; Accepted: 14 February 2020; Published: 17 February 2020

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Abstract: As measurements are expensive and laborious, the estimation of soil hydraulic properties using pedotransfer functions (PTFs) has become popular worldwide. However, the estimation of soil hydraulic properties is not the final aim but an essential input value for other calculations and simulations, mostly in environmental and crop models. This modeling approach is a popular way to assess agricultural and environmental processes. However, it is rarely used in Sri Lanka because soil hydraulic data are rare. We evaluated the functionality of PTFs (developed to estimate field capacity (FC) and the permanent wilting point (PWP) of Sri Lankan soils) for process-based crop models. We used the Agricultural Production Systems sIMulator (APSIM) as the test model. Initially, we confirmed the importance of PWP (LL15) and FC (DUL) by assessing the sensitivity of the soil input parameters on the growth and yield of rice under rainfed conditions. We simulated the growth and yield of rice and the four selected outputs related to the APSIM soil module using the measured and estimated values of FC and PWP. These simulations were conducted for ten years in 16 locations of Sri Lanka, representing wet, intermediate, and dry zones. The simulated total aboveground dry matter and weight of the rough rice, using both input conditions (the measured and PTF-estimated soil hydraulic properties), showed good agreement, with no significant differences between each other. Outputs related to the soil module also showed good agreement, as no significant differences were found between the two input conditions (measured and PTF-estimated soil hydraulic properties). Although the DUL and LL15 are the most influential parameters for the selected outputs of APSIM–Oryza, the estimated FC and PWP values did not change the predictive ability of APSIM. In this way, the functionality of PTFs for APSIM crop modeling is confirmed.

Keywords: APSIM; rice; sensitivity analysis; simulation; soil hydraulic properties

1. Introduction

The direct measurement of some soil hydraulic properties is laborious and expensive. Hence, information about soil hydraulic properties at an appropriate scale is limited in most parts of the world, especially in tropical regions [1]. Pedotransfer functions (PTFs) are predictive functions used to estimate difficult-to-measure soil parameters with easily measurable soil parameters [2]. Point-based PTFs are used to determine soil parameters at specific, conventional values of matric potential [3]. The moisture content at −10 and −33 kPa (representing the field capacity (FC)) and moisture content at –1500 kPa (representing the permanent wilting point (PWP)) are the most common reference values for the soil moisture characteristic curve (SMCC) used for point PTFs [4].

Point PTFs were developed [5] for Sri Lankan soil and confirmed the statistical accuracy of these PTFs for Sri Lankan conditions. However, these PTFs cannot perfectly calculate soil hydraulic parameters. In other words, there are always some errors that could be over or underestimated according to soil type. These errors may be different according to the application of the PTFs. Hence, the final estimation of the model quality should be defined by the model's applicability [6] because the estimation of hydraulic properties is not the final aim. Instead, these properties are essential inputs for other calculations and simulations [7]. Wosten et al. [7] proposed to use a functional criteria analysis, which evaluates the functional behavior of estimated parameters in different applications. Subsequently, a functional analysis (or functional criteria analysis) was carried out to determine the performance of the estimated parameters on different applications [7–9]. However, this type of analysis is rarely used for process-based crop models. A functional analysis, coupled with a stochastic model of the soil hydraulic parameters, can be effectively employed to assess the relative performance of different parameterization methods by evaluating how model parameter uncertainties propagate through the stochastic model [10,11]. Some authors have discussed the importance of functional analysis for the uses of PTFs and have reported the importance of functionally evaluating PTFs for real field-scale applications [7,9,12,13].

One of the most popular applications of PTFs is using model simulations for environmental and crop processes. Studies have been conducted to evaluate the functionality of PTFs for environmental simulations, such as water flow simulations [13–17], evapotranspiration simulations, water balance studies [10,11,18,19], and irrigation water estimations [5,20], using different models. However, no such comprehensive studies have been conducted for process-based crop models [5].

Process-based crop models derive their output based on soil, climate, plant, and management parameters; therefore, the accuracy model output depends on the accuracy of the input parameters. At present, the acquisition of historic climate information for specific locations is easy due to the availability of ground-level observations and grid-based generated datasets. Similar performances of gridded climatic data and observed data in yield predictions using process-based crop models have been reported [21–23]. Therefore, ground-level observations may be successfully replaced with grid-based generated data. However, knowledge of soil parameters is crucial, as these parameters are largely responsible for the variability of process-based crop model outputs [24–26] and are often taken from nearby soil surveys or expert knowledge. However, due to its inherent variations, this information may need to be acquired at a finer scale for better estimations using process-based crop models [25].

Crop modeling aims to describe and understand the relevant plant processes and their interactions with abiotic and biotic factors [27]. Agricultural Production Systems sIMulator (APSIM) [28], Decision Support Systems for Agrotechnology Transfer (DSSAT) [29], and Simulateur mulTIdisciplinaire pour les Cultures Standard (STICS) [30] are some of the most widely used dynamic crop models to analyze agricultural processes under different input parameters, such as abiotic and biotic factors, crop parameters, and management conditions. However, APSIM has been applied widely because it has a user-friendly interface with advanced flexibility in establishing simple and complex simulations [31].

APSIM is an open-source (for non-commercial uses) crop modeling software that can be used to model the growth and yield of many crops [28,32]. This model is driven by daily climate data and can simulate the growth, development, and yield of crops and their interactions with soil and management conditions. Further, it includes modeling functions that allow one to simulate the soil water, nutrients, and much more. Plant models in APSIM simulate major physiological processes, such as phenology, water, and nutrient uptake, the development of organs and responses to abiotic stresses, etc. The soil module in APSIM simulates water movements, such as infiltration, capillary rise, evaporation, surface runoff, and drainage [28,32]. APSIM requires soil hydraulic inputs, such as the drained upper limit (DUL), drained lower limit, and crop lower limit (LL15 and crop LL), saturation (SAT), hydraulic conductivity (KS), and drainage coefficient (SWCON), for its simulations. It also uses some soil physicochemical parameters, such as soil bulk density (BD), organic carbon percentage (OC), pH, and the initial nutrient levels for simulations. Since the level of influence of these parameters may be different, it is vital to study the influence of these parameters on the model output using sensitivity analysis [33,34]. Sensitivity analyses are used to evaluate the responses of model outputs to changes in model input parameters and to quantify the relative importance of those responses [35,36]. Many studies have been conducted to evaluate the sensitivity of plant parameters and the management practices of different crops under different models [24,37–43]. Although the sensitivity assessment of soil is essential [25], limited attention has been paid to evaluating the sensitivity of soil parameters [42]. Hence, this study aims to evaluate the sensitivity of soil parameters to the growth and yield of rice using the APSIM–Oryza model in APSIM 7.10.

Gunarathna et al. [5] developed point PTFs to estimate the FC and PWP of Sri Lankan soils. Although they reported statistical validity, no comprehensive studies were conducted to test the functionality of these PTFs.

In this study, we aimed to assess the functionality of these PTFs for process-based crop models. We compared the rice growth and yield with different soil input conditions (such as measured soil data and PTF-estimated soil data) to assess the functionality of PTFs for APSIM–Oryza simulations under tropical Sri Lankan conditions. At first, we conducted a sensitivity analysis to confirm whether the parameters calculated by PTFs are sensitive in a simulation using APSIM–Oryza. Then, we confirmed the statistical agreement between the simulations using the measured soil data and calculated soil data with the PTFs. Moreover, we examined the required improvements of the PTFs to simulate the yield more accurately.

2. Materials and Methods

As a staple food, rice is the most commonly grown agricultural crop and accounts for 34% of the total cultivated area of Sri Lanka. Considering the social, cultural, and economic importance of rice, many studies (including crop modeling) have focused on the rice production systems of Sri Lanka. Hence, we selected rice to study the functionality of the developed PTFs in process-based crop models, particularly using APSIM version 7.10. Rice cultivation requires a vast amount of water. Consequently, rice is extremely vulnerable to drought damages due to the high spatial and temporal variation of the rainfall in Sri Lanka. In Sri Lanka, rice is cultivated in two major seasons (known as *Maha* and *Yala*) based on rainfall distribution and water availability [44]. In the *Maha* season (October to March), primarily rainfed rice cultivation is practiced in the lowlands with or without supplementary irrigation. In the *Yala* season, rainfed rice cultivation is limited due to low rainfall and irrigated rice cultivation is only practiced where irrigation is possible. Therefore, we ignored the *Yala* season (April to September) and rainfed rice cultivation in the *Maha* season (without supplementary irrigation) for this simulation study. The elements of this study are twofold [6]:

I. Sensitivity analysis is used to confirm the influential ability of FC and PWP for the outputs of the APSIM–Oryza model;

II. A study of the functionality of PTFs is developed to estimate FC and PWP for APSIM crop modeling.

For the sensitivity analysis, we selected three locations (1–3) representing the three climatic zones of Sri Lanka (a wet zone, with a mean annual rainfall of > 2500 mm, a dry zone with a mean annual rainfall of < 1750 mm, and an intermediate zone, with a mean annual rainfall of 1750–2500 mm), while 16 locations (including the above-mentioned three locations) were selected for the functional analysis (Figure 1). For both parts of the analysis, the required APSIM files were prepared as follows.

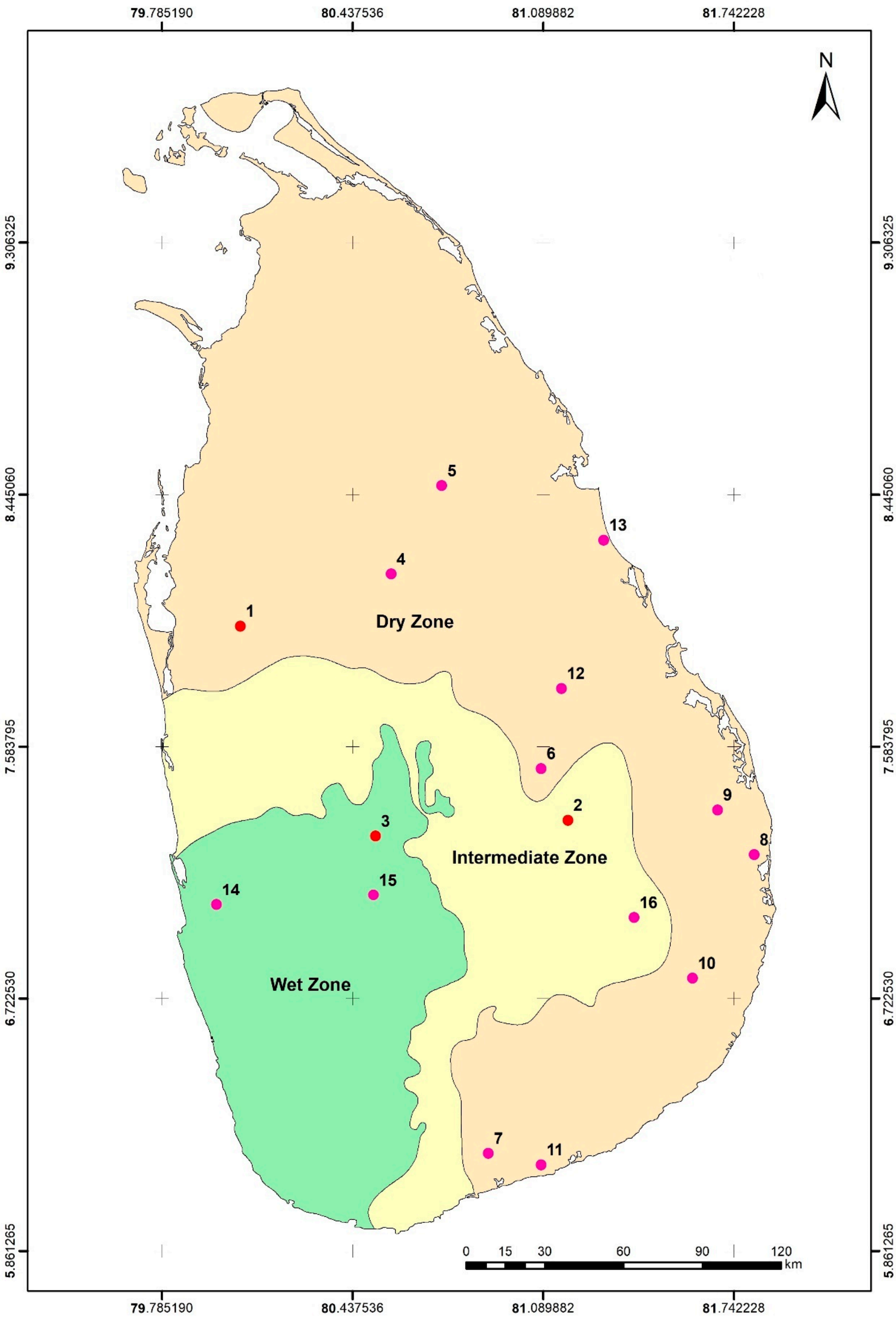

Figure 1. A map of Sri Lanka showing the study sites and climatic zones defined based on the mean annual rainfall.

2.1. Meteorological Data

The AgMERRA climate forcing dataset provides daily, high-resolution meteorological data for the period of 1980–2010. We extracted the daily rainfall, maximum temperature, minimum temperature, and solar radiation of 16 selected locations from the AgMERRA global gridded climate dataset [45,46] using the NetCDF-Extractor V2.0 tool of AgriMetSoft (https://www.agrimetsoft.com).

2.2. Soil Data

The factsheets of the Sri Lankan, Canadian Soil Resource (SRICANSOL) project of the Soil science society of Sri Lanka contain a comprehensive dataset of Sri Lankan soils, including information on land use, as well as taxonomic, physical, and chemical properties [5,47–49]. This dataset includes information at the soil horizon level; therefore, the depth of the layers varies from location to location. We used the SRICANSOL database to prepare soil profiles of the above-mentioned 16 locations. We considered the depth of different soil horizons as the depth of the layer of the soil profiles. We collected information on the soil pH, organic carbon (OC), bulk density (BD), and moisture content of −33 kPa (DUL) and −1500 kPa (LL15) saturated hydraulic conductivity (KS) to develop soil profiles for the pertinent locations. The crop LL was considered to be similar to LL15. Other than the aforesaid measured data, air drying (considered as half of LL15) and saturation (considered as equal to the porosity) were also used as input parameters. Porosity (n) was calculated using the following equation, assuming 2.65 g/cm^3 as the true density (TD). BD denotes the bulk density in Equation (1).

$$n = 1 - \frac{BD}{TD} \quad (1)$$

Gunarathna et al. [5] used point PTFs to estimate volumetric water contents using the multiple linear regression method. They developed PTFs to estimate volumetric water contents at −33 and −1500 kPa, representing the field capacity and permanent wilting point using various levels of input parameters. Considering their practical importance, the PTFs developed to estimate −33 and −1500 kPa, using the sand percentage of soil (Equation (2) and (3)), were used to estimate the DUL and LL15 for the input uncertainty assessment due to the parameter estimation using PTFs. We duplicated the above-mentioned 16 soil profiles and modified them by changing their respective PTF-estimated DUL (VWC33) and LL15 (VWC1500) values. Air-dried and crop-LL values were also modified accordingly.

$$\mathrm{VWC33} = 0.4357 - 0.035 \times \mathrm{Sand\%} \quad (2)$$

$$\mathrm{VWC1500} = 0.3426 - 0.003 \times \mathrm{Sand\%} \quad (3)$$

2.3. APSIM Simulation

APSIM is a process-based dynamic crop model that combines biophysical and management modules within a central engine to simulate diverse cropping systems [28,32]. To model crop growth, we used specific modules linked to the engine of APSIM, such as the specific crop model (APSIM–Oryza) and the soil water module (SOILWAT). The APSIM-crop model simulates crop-growth processes using the information on water from the SOILWAT module. APSIM uses the Oryza model [50,51] to simulate the daily rate of dry matter production and the phenological development of rice plants under different environments, including the ponding conditions [50].

The simulation of soil and crop variables started on 1 April of the year 2000 and continued until 31 December 2010, as this period represents dry, wet, and normal years. We considered the rice direct-seeding for this simulation, as it is the most common practice of field establishment for rice crops in Sri Lanka [52]. The cultivation decisions of Sri Lankan rainfed rice farmers are dependent on the onset of rainfall [52]. In simulations, we sowed rice when 20 mm of rainfall was accumulated over three days between November 15 to 30 or on December 1 in each year from 2000 to 2009. Considering the regular practices of Sri Lankan rice farmers, the planting density was set as 180 plants per square meter. We selected the Sri Lankan local cultivar BG357 for this study. We modified the Oryza model in APSIM 7.10 by adding the new cultivar BG357 and parameterized the cultivar using the values reported by Zubair et al. [53] and Nissanka et al. [54]. We set the maximum ponding as 100 mm during the period of 1 December until the end of February. Considering the fertilizer recommendations of the Department of Agriculture-Sri Lanka for rainfed rice, we set the fertilizer application to 30, 45, and 20 kg for the Urea nitrogen per hectare at 14, 28, and 42 days after the emergence, respectively. We assumed all the other management practices, including weed control, pest, and disease control, would follow the standard management practices recommended by the Department of Agriculture. We selected the total above-ground dry matter (WAGT) (kg/ha) and dry weight of rough rice (WRR) (kg/ha) as the output variables for this simulation study.

2.4. Sensitivity Analysis

Sensitivity analysis is (SA) a type of informative analysis used to determine which input parameter/s had the most influence on the model output. However, the purpose of the SA in this study was to confirm the influence of the parameters estimated by PTFs using the simulation of APSIM–Oryza. The SA could be local or global, according to the strategy used to explore the parameter space. Local methods could be relatively easily implemented and also require low computational costs compared to global methods. However, these methods have some shortcomings, including the inability to detect interactions between parameters and a heavy dependence on the base values of the input parameters [35,55]. A global sensitivity analysis overcomes the demerits of local methods, as it explores the entire multi-dimensional parameter space simultaneously. Hence, for a specific output variable, the influence of single parameters, as well as the interactions between parameters can be evaluated [35]. However, his process is computationally expensive, especially for process-based complex models [56].

An emulator is a simplified statistical approximation of a more complex model [57] used as a substitute for computationally expensive models. An emulator with sufficient accuracy can successfully replace an actual simulator to perform a sensitivity analysis [58]. In this emulator-based approach, a simulator that runs for a relatively smaller number of simulations could be used to build the emulator; then, the emulator could be used for the sensitivity analysis. Many studies used the GEM-SA software for sensitivity analyses of different process-based complex models [56,59–62]. Kennedy and O'Hagan [63]; Kennedy et al. [64]; and Kennedy and Petropoulos [59] reported a full description of the underlying mathematical procedures used in the GEM-SA software.

In this study, eight soil parameters (Table 1) were selected to study the sensitivity of the total above-ground dry matter (WAGT) and dry weight of rough rice (WRR) to rice crops under rainfed conditions. Initially, we generated 300 test points representing the entire range of respective inputs and related outputs (WAGT and WRR) of the APSIM simulator using the APSIM-R package [65] of the R software [66]. When generating 300 test points, the ranges were set by considering the typical ranges of Sri Lankan soils (Table 1). In this study, we used the Gaussian Process (GP) emulator in the the GEM-SA software [64] to develop 60 emulators (10 years × 2 outputs × 3 environments). Kennedy and O'Hagan [63]; Kennedy et al. [64]; and Kennedy and Petropoulos [59] offer a more detailed discussion of the analytical procedures of GEM-SA. In this study, we estimated the main effects and sum effects, assuming that all input uncertainties are unknown but uniform [62]. Further, we set the prior mean option as linear for each input [62]. We assessed the models using the leave-one-out cross-validation procedure embedded in GEM-SA [62]. With leave-one-out cross-validation, the emulator was used to estimate the emulator variance of each of the training runs in turn [59]. A slightly modified emulator was used to estimate each training point using all other training points. The GEM-SA calculates several diagnostics, including the sigma square value, cross-validation root mean squared error (CV-RMSE), and cross-validation root mean squared standardized (CV-RMSSE) using the results of the cross-validation [59]. These diagnostics could be used to assess the accuracy of the emulator approximations. The sigma squared value also provides a better understanding of the emulator accuracy. In this study, we evaluated the emulator accuracy using the above built-in diagnostic options of GEM-SA [62].

$$CVRMSE = \sqrt{\frac{\sum_{i=1}^{n} (y_i - \hat{y})^2}{n}} \tag{4}$$

$$CVRMSSE = \sqrt{\frac{\sum_{i=1}^{n} ((O_i - \hat{y})/s_i)^2}{n}} \tag{5}$$

where y_i is the true output for the ith training run, $\hat{y}$ is the corresponding emulator approximation, s_i is the standard deviation calculated with the ith training point removed, and n is the number of runs [59,62].

Table 1. Selected soil parameters for the sensitivity analysis.

Parameter	Description	Unit	Range	
			Min	Max
BD	Bulk density	g/cm^3	0.8	2.0
LL15	Drained lower limit (equals the permanent wilting point)	mm/mm	0.05	0.30
DUL	Drained upper limit (equals the field capacity)	mm/mm	0.0 *	1.0 *
SAT	Saturation	mm/mm	0.0 **	1.0 **
KS	Saturated hydraulic conductivity	mm/day	0.1	10,000
OC	Organic carbon	%	0.1	1.5
pH			4.0	9.0
SWCON	Drainage coefficient		0	1

* Change according to the LL15 and SAT; ** Change according to the BD, LL15, and DUL.

The variance-based sensitivity index (main effect, S_{i}) was estimated by partitioning the output variance induced by the variations in all input parameters under the assumption that all input uncertainties are unknown but uniform. S_i represents the expected reduction in the output variance if parameter x_i is known [61,62], and the relative importance of each parameter in terms of its effect on output uncertainty can be ranked using the S_i values of the selected parameters [67]. The main effect index (Si) is defined as

$$S_i = \frac{Var\{E(f(X|x_i)\}}{Var\{f(X)\}} \tag{6}$$

where $Var\{f(X)\}$ is the total variance in the output, given variations in all parameters, and $Var\{E(f((X\,|\,x\_i)\}$ is the variance in the expected output f(X) if x_i is known.

2.5. Functional Analysis

We simulated the total above-ground dry matter (WAGT) (kg/ha) and the dry weight of rough rice (WRR) (kg/ha) for the BG357 cultivar of rice for the 16 selected locations. At first, we used the soil profiles developed using the measured soil data (hereafter known as the "measurement-based simulation"). Then, we modified the soil profiles by changing the DUL and LL15 using the PTF-derived values. Further, the air-drying (half of LL15) was also modified accordingly. Secondly, we simulated the WAGT and the WRR of BG357, the cultivar of rice for all 16 locations using the modified soil profiles (hereafter known as 'PTF-based simulation'). We compared the results of both measurement-based and PTF-based simulations to study the effects of input uncertainty on the model outputs.

Four selected outputs of the APSIM soil module (daily infiltration (infiltration), daily runoff (runoff), the soil water content of the topsoil layer (SWS(1)), and the potential evapotranspiration after modification for green cover and residue (EOS)) were also simulated for both soil profiles and compared.

A simple linear regression was used to compare the paired data points obtained for the measurement-based and PTF-based simulations. Further, we checked the results of the variances and then evaluated them using a t-test assuming unequal variances. The root mean square error

(RMSE) (Equation (6)), a widely used measurement to study the goodness of fit of observations and estimations [68], was used for this study. Nash–Sutcliffe efficiency (NSE) (Equation (7)) [69], the efficiency calculated as one minus the sum of the absolute squared differences between the predictions and the observations normalized by the variance of the observations [70], was also used to evaluate the goodness of fit of the two estimations. The index of agreement (d) (Equation (8)), a standardized measure of the degree of the model prediction errors, which varies between 0 (no agreement) and 1 (perfect fit) [71], was also used to study the goodness of fit of the observations and estimations.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (S_i - O_i)^2}{n}} \tag{7}$$

$$NSE = 1 - \frac{\sum_{i=1}^{n} (O_i - S_i)^2}{\sum_{i=1}^{n} O_i - \overline{O})^2} \tag{8}$$

$$d = 1 - \frac{\sum_{i=1}^{n} (S_i - O_i)^2}{\sum_{i=1}^{n} \left(\left|S_i - \overline{O}\right| + \left|O_i - \overline{O}\right|\right)^2} \tag{9}$$

where S_i is the simulated value, O_i is the observed value, and $\overline{O}$ is the mean of the observations.

The Lin's concordance correlation coefficient (CCC) integrates precision using Pearson's correlation coefficient—which represents the proportion of the total variance in the observed data that can be explained by the model, and accuracy with bias—which indicates how far the regression line deviates from the concordance line [72]. The CCC ranges from −1 to 1, with a perfect agreement at 1. According to the CCC, this agreement could be classified as almost perfect (>0.99), substantial (0.95–0.99), moderate (0.90–0.95), or poor (<0.90) [73]. This method can legitimately calculate accuracy with few observations for agreement using a continuous measure obtained by the two methods [74]. We calculated the CCC using the epiR package [74] in the R software [66].

3. Results and Discussion

3.1. Sensitivity Analysis

First, we evaluated the accuracy of the emulators. The sigma squared value, a measure of the nonlinearity of the emulator, records values near zero when an emulator model shows linearity. It shows higher values when the emulator models show moderate or high nonlinearity; however, no cut off values were reported to explain the linearity or nonlinearity. Petropoulos et al. [56] reported that their emulators showed linearity or moderate nonlinearity when they recorded sigma squared values between 0.13 and 1.6. Gunarathna et al. [62] reported sigma squared values between 0.10 to 1.43, reported as good to moderate linearity. In this study, we observed sigma squared values between 0.02 and 0.48 (Appendix Tables A1 and A2); hence, we confirmed the linearity of the emulator models, though no clear cutoff values were determined to define the linearity. The CV-RMSE values reported far lower values compared to the standard deviation of the simulator results. Thus, we confirm that the results of the emulator are close to the simulator results (Appendix Tables A1 and A2). CV-RMSSE shows values near one when the emulator results are close to the simulator results, while higher and lower values indicate over and underestimations, respectively. The CV-RMSSE values were between 0.92 and 1.26 (Appendix Tables A1 and A2). All of these diagnostics reported comparatively better values than the previously reported values of the emulator accuracy assessments, which were reported to be satisfactory emulators [56,59,62,75].

Figure 2 shows a boxplot diagram for the sensitivity index of the eight parameters selected for the model outputs (total above-ground dry matter (WAGT) (kg/ha) and the dry weight of rough rice (WRR) (kg/ha)). The results revealed that DUL is the most influential parameter for the simulation of WAGT and WRR for rice crops, while LL15 showed the second-highest sensitivity to the selected outputs. SWCON and SAT also showed slight sensitivity to the selected outputs. All other selected parameters recorded low sensitivity indices; hence, BD, OC, KS, and pH were identified as less-sensitive soil parameters for WAGT and WRR.

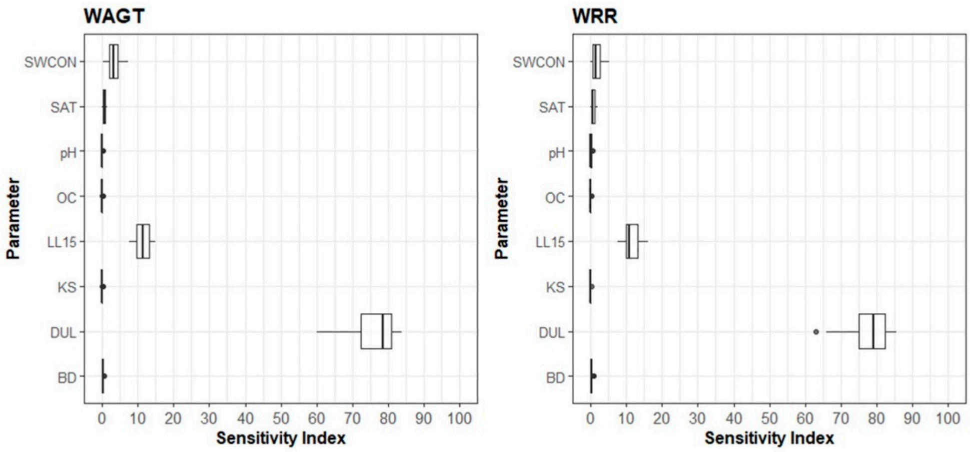

Figure 2. Variation of the the sensitivity index (*Si*) of selected soil parameters on the simulated total above-ground dry matter (WAGT) and simulated dry-weight of rough rice (WRR) for rice in Sri Lanka.

Similarly, Varella et al. [25] showed a higher sensitivity of field capacity when simulating the growth and yield of wheat and sugar beet using the STICS model. Chen et al. [76] also showed a higher sensitivity of wheat yield to the available water capacity.

The results confirm that DUL and LL15 are the most critical soil parameters for APSIM–Oryza model simulations. Hence, an accurate estimation of DUL and LL15 is of prime importance in APSIM–Oryza simulations compared to other selected soil parameters. SWCON and SAT also showed little sensitivity to the output; hence, a reliable method is required to estimate SWCON with reasonable accuracy. Further, a reasonable estimation of the SAT may help increase the accuracy of the simulations. Other selected soil parameters, such as BD, OC, pH, and KS, showed the lowest sensitivity for the selected model outputs. Hence, a rough estimation of these parameters may not contribute significant changes to the outputs. However, the estimation of most of those parameters is not laborious or expensive compared to DUL and LL15.

3.2. Functional Analysis

Few studies have reported on the development of PTFs for tropical Sri Lankan soils, such as an evaluation of existing PTFs [77] and developing PTFs to estimate PWP and FC [5,78]. In this study, we checked only the functionality of PTFs developed to estimate FC and PWP [5] because no empirical equations have been developed to estimate other soil parameters. However, these values may not significantly affect the outputs because the sensitivity of these parameters remains low compared to DUL and LL15. We used the measured parameters as the other input variables (except crop LL and air dry), neglecting the uncertainty of those parameters.

Measurement-based simulations showed a strong relationship with PTF-based simulations for rice crop growth and yield using the APSIM–Oryza model (Figure 3). Further, the selected outputs of the APSIM soil module (daily infiltration (infiltration), daily runoff (runoff), soil water content of the topmost soil layer (SWS(1)), and potential evapotranspiration after modification for green cover and residue (EOS)) also showed good agreement between measurement-based and PTF-based simulations (Figure 3).

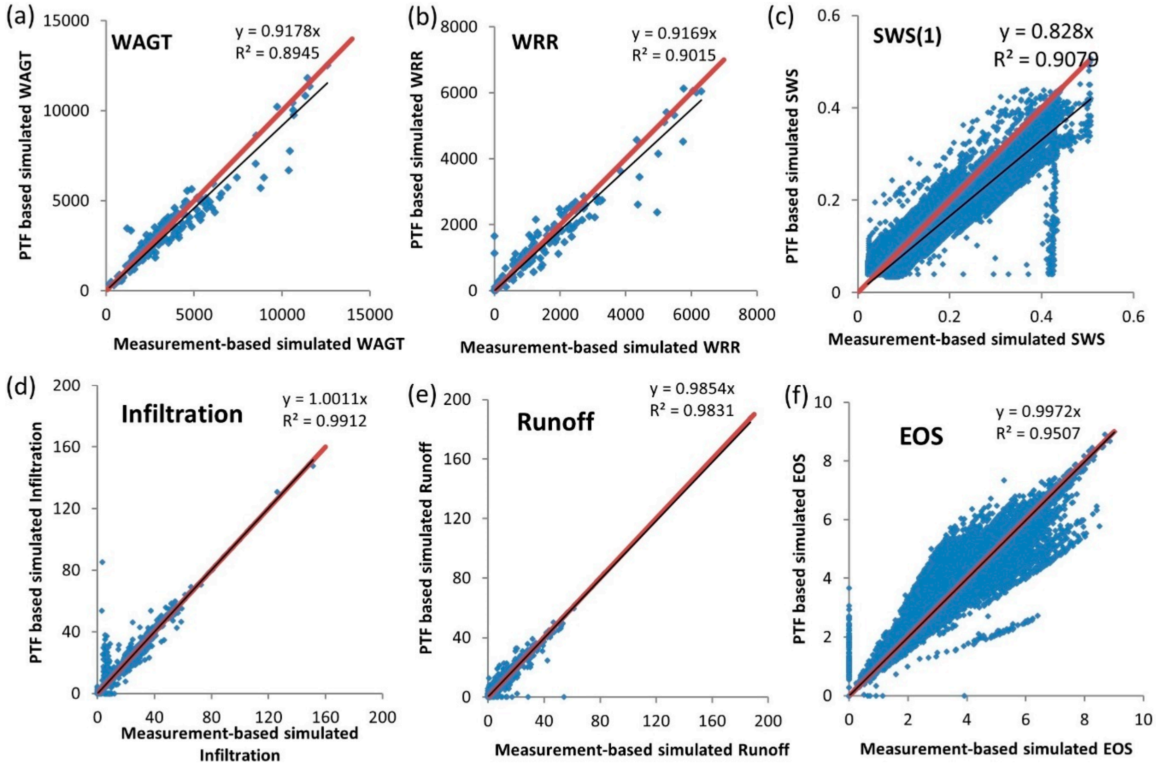

Figure 3. Relationship between use of measurement-based inputs and pedotrandfer functions derived (PTF-based) inputs on simulations of rice, (**a**) Total above-ground dry matter (WAGT) (kg/ha) of rice; (**b**) Dry weight of rough rice (WRR) (kg/ha); (**c**) Soil water content of the topsoil layer (SWS(1)) (mm/mm); (**d**) Daily infiltration (infiltration) (mm); (**e**) Daily runoff (runoff) (mm); and f) Potential evapotranspiration after modifications of green cover and residue (EOS) (mm).

Measurement-based and PTF-based simulations showed 0.89 and 0.90 R^2 values for WAGT and WRR, respectively (Table 2). This ensures no significant differences between PTF-based simulations and measurement-based simulations. A comparison between the outputs of the rice simulations (WAGT and WRR) under both simulation scenarios also confirmed the acceptability of PTF-based simulations, as no significant difference ($p > 0.05$) between both types of simulations under a t-test was observed (Table 2). The reported Nash–Sutcliffe efficiency was 0.89 and 0.90 for WAGT and WRR, respectively. Hence, we confirmed the similarity of PTF-based and measurement-based simulations. Wilmott's index of agreement also confirmed the agreement of the results of PTF-based simulations with measurement-based simulations for both WAGT (d = 0.97) and WRR (d = 0.99). The RMSEs for WAGT and WRR were 811 and 445 kg/ha, respectively, which also confirmed the similarity of both simulation scenarios, which were assumed to be within the bounds (half of the standard deviation (SD) of the measurement-based simulations) (WAGT, SD = 2485 kg/ha; WRR, SD = 1424 kg/ha).

Table 2. Performance evaluation of the simulation accuracies of the measurement-based and PTF-based simulations.

Criteria	WAGT	WRR	SWS(1)	Infiltration	Runoff	EOS
R^2	0.90	0.90	0.91	0.99	0.98	0.95
RMSE	811 kg/ha	445 kg/ha	0.05 mm/mm	0.74 mm	0.45 mm	0.35 mm
NSE	0.89	0.90	0.85	0.99	0.98	0.95
d	0.97	0.97	0.95	1.00	1.00	0.99
CCC	0.94	0.95	0.91	1.00	0.98	0.99
SD	2485 kg/ha	1424 kg/ha	0.12 mm	7.84 mm	3.47 mm	1.63 mm
P(T <=t)	0.42	0.60	0.06	0.83	0.74	0.02

WAGT: Total above-ground dry matter of rice (kg/ha), WRR: Dry weight of rough rice of rice (kg/ha), SWS (1): Soil water content of the topsoil layer (mm/mm), infiltration: Daily infiltration (mm), runoff: Daily runoff (mm), EOS: Potential evapotranspiration after modification for green cover and residue (mm); R^2: Coefficient of determination, RMSE: Root mean square error, NSE: Nash–Sutcliffe efficiency, *d*: Index of agreement, CCC: Lin's concordance correlation coefficient, *SD*: Standard deviation, *P*: Probability of t-test.

The measurement-based and PTF-based simulations showed over 0.90 each for the R^2 values for all selected soil module related daily outputs (SWS(1), Infiltration, Runoff, and EOS) (Table 2). This ensures that PTF-based simulations can perform as well as measurement-based simulations. Further, the comparison of soil module related outputs between both simulation scenarios also confirmed the acceptability of PTF-based simulations, as no significant difference ($p > 0.05$) was found between both simulation scenarios for infiltration and runoff (Table 2). The Nash–Sutcliffe efficiency showed a better agreement between the two simulation scenarios, as all outputs related to the soil module recorded an NSE over 0.85. Wilmott's index of the agreement also confirmed the agreement of the results of the PTF-based simulation with the measurement-based simulation for all soil module related outputs, reporting over 0.95 for d. The RMSE for SWS(1), Infiltration, Runoff, and EOS were 0.05 mm/mm, 0.70 mm/day, 0.45 mm/day, and 0.35 mm/day, respectively, which also confirmed the similarity of both simulation scenarios, which were assumed to be within the bounds.

This result proved the ability of PTF-based soil profiles to simulate WAGT, WRR, SWS(1), infiltration, runoff, and EOS reasonably equally to the measured soil profiles. As both parameters derived using PTFs are the soil parameters most sensitive to the growth and yield of rice, the functionality of PTFs are remarkable for APSIM crop modeling. Therefore, PTF-based estimations of DUL and LL15 may provide a solution for the data unavailability for crop and environmental simulation purposes. As measuring LL15 and DUL is laborious and expensive, the application of PTF to develop soil profiles may help cut down unnecessary expenses and delays.

There are no studies on functionality assessments for crop models. Moeys et al. [13] conducted a functional assessment to check the reproducibility of PTF-estimated soil parameters to predict water flow and solute transport. They reported the capability of PTF to be reasonably good, with reported CCC values of 0.54–0.72. In this study, we observed CCC values from 0.91 to 1.00.

We confirmed the statistical agreement between the APSIM simulation with measured soil parameters and APSIM simulation with PTF-estimated soil parameters. However, WAGT, WRR, and SWS(1) showed a slight underestimation of PTF-based simulations compared to the measurement-based simulations. Hence, it is important to study the causes of underestimation and the possibility to minimize these underestimations for precise modeling assessments.

Figure 4 shows that the developed PTFs slightly underestimated the LL15 and DUL of the selected Sri Lankan soils. The underestimation of DUL and LL15 in the PTF estimations may be attributed to an underestimation of the yields.

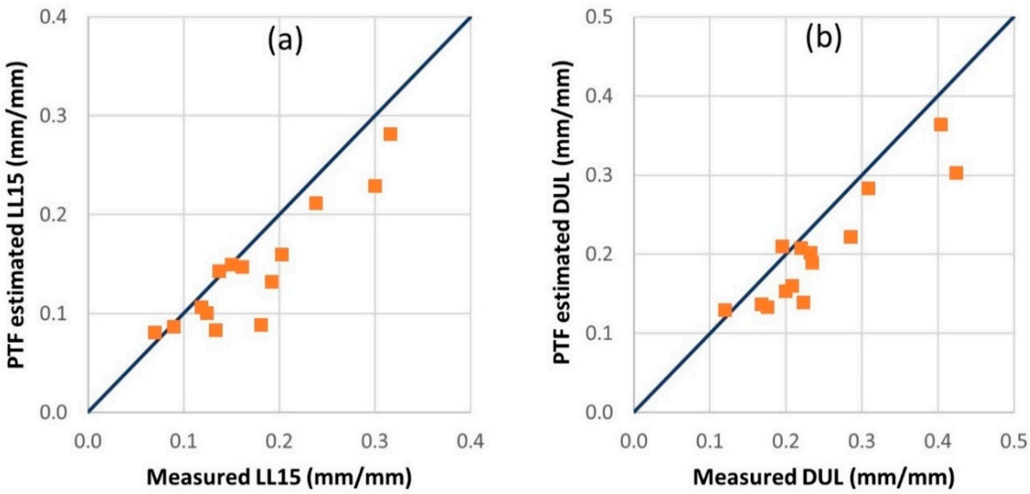

Figure 4. Relationship between the measured and PTF-estimated soil hydraulic parameters (whole soil profile) of the selected soil profiles; (**a**) lower limit (LL15) and (**b**) drainage upper limit (DUL).

We assessed the accuracy of PTFs using CCC. The CCC values for LL15 and DUL were 0.81 and 0.79, respectively, which were classified as poor [73]. Figure 5 shows the average (2000–2010) *maha* season WAGT and WRR of the 16 selected locations. The estimated WAGT and WRR showed substantially higher CCC values (0.95 and 0.97 for WAGT and WRR, respectively, which is classified as substantial [73]), thereby confirming a relationship close to 1:1 between the measurement-based simulations and the PTF-based simulations. Nasta et al. [11] conducted a functional assessment of PTFs to predict the soil water budget. They reported the poor performances of the water budget assessment (NSE = 75%) compared to the PTF-estimated variables (NSE = 85%). Therefore, we can conclude that the functionality of PTF is remarkable for APSIM simulations. Nemes et al. estimated the irrigation water requirement [20] and water transport modeling [79] using measured and PTF-estimated soil hydraulic parameters and reported the similarity of both input conditions. Gunarathna et al. [5] also reported the similar irrigation water estimations using PTF-based and measurement-based soil hydraulic data estimations. However, no details on the accuracy assessment have been reported.

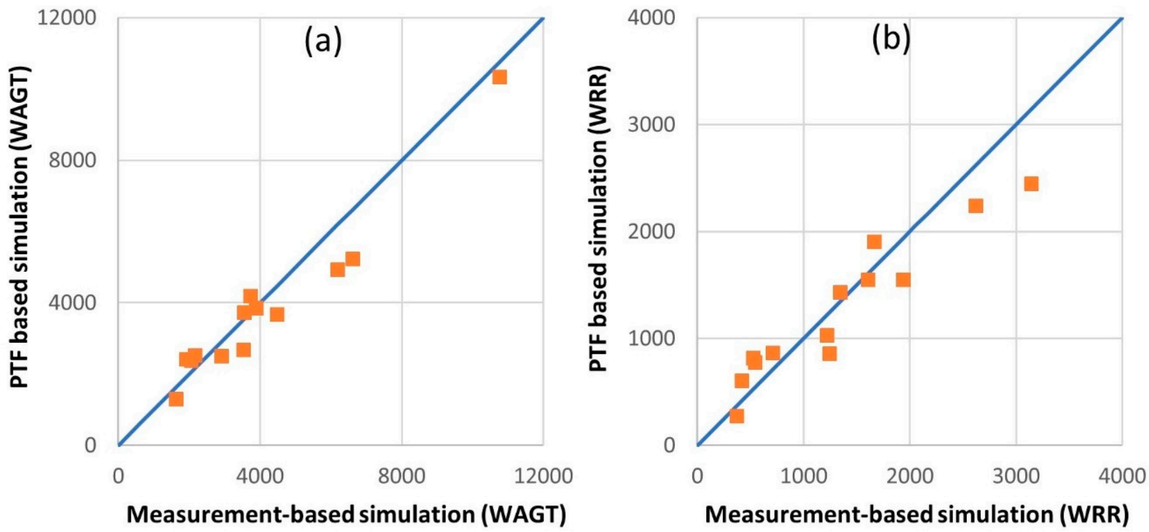

Figure 5. Relationship between measurement-based and PTF-based simulations of average yields (2000–2010); (**a**) The total above-ground dry matter of rice (kg/ha); WAGT, (**b**) dry weight of rough rice (kg/ha); WRR.

Figure 6 shows the error variations of the different locations of PTFs and PTF-based simulations. The blue and red parts of the graph represent the overestimation and underestimation of AWC (DUL-LL15), respectively. From these graphs, we can confirm that the underestimation of AWC may cause underestimation of the yield (WAGT and WRR), and the overestimation of AWC may cause overestimation of the yield. The underestimation of AWC's influence can also be confirmed. Since the DUL is most sensitive in the APSIM simulation, the improvement of the PTF with DUL may be important for more accurate APSIM simulations.

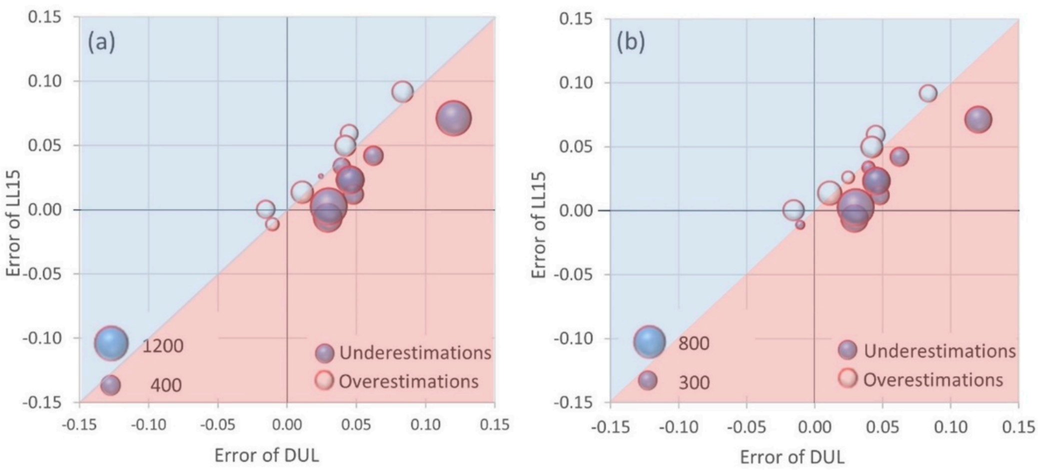

Figure 6. The error variation of PTF-based simulations of average yield (2000–2010) in different locations; (**a**) total above-ground dry matter (kg/ha); WAGT and (**b**) weight of rough rice kg/ha; WRR; LL15: Lower limit (mm/mm), DUL: drainage upper limit (mm/mm); The size of the bubble represents the magnitude of the error of the estimated yield.

In most locations, both LL15 and DUL showed underestimations (Figures 4 and 6). However, in PTF-based APSIM simulations, WAGT and WRR showed both overestimations and underestimations but without any patterns. Hence, the error distribution is random, confirming that the effect of the regular underestimation (of hydraulic parameters) by the PTFs developed by Gunarathna et al. [5] did not appear in the output of the APSIM yield simulations. In this way, the functionality of PTFs on APSIM simulations is further confirmed.

4. Conclusions

Among the soil input parameters, the APSIM–Oryza model is highly sensitive to the drained upper limit and drained lower limit and is moderately sensitive to the drainage coefficient and saturation. Therefore, the proper estimation of those parameters is vital to the growth and yield simulations of rice using the APSIM–Oryza model.

The characterization of the sensitivity of the model input parameters to the model outputs has essential implications for model design and interpretation, as well as for future data collection efforts. Therefore, the results of these sensitivity analyses can be used as a guide for future crop modeling research work.

Despite the higher sensitivity levels of the drained upper and lower limits, the simulated PTF-based soil profiles were comparable to the measurement-based soil profiles. As the variability in the simulated yields using PTF-based soil profiles is within the expected limits, the PTF can be considered a better model; we conclude that PTF-based estimations of the drained upper limit and lower limit can be successfully used to simulate crop growth and yield under similar environments. Hence, the functionality of PTFs for APSIM simulations has been confirmed, and the laborious and expensive measurements of drained upper and lower limits can be successfully replaced by PTF estimations.

5. Limitations

Due to data limitations, we used gridded climatic data for this study without any proper validation before using them. However, this may not significantly affect our results, as we compared two simulations using the same climatic data. Although the use of the gridded data has been validated in other environments, it is not yet validated in Sri Lanka; therefore, we suggest conducting studies to check the applicability of gridded climatic data for crop modeling studies.

Author Contributions: Conceptualization, M.H.J.P.G. and K.S.; data curation, M.H.J.P.G. and M.K.N.K.; formal analysis, M.H.J.P.G. and M.K.N.K.; methodology, M.H.J.P.G., M.K.N.K., and M.R.; supervision, K.S.; writing—original draft, M.H.J.P.G. and M.K.N.K.; Writing—review and editing, M.H.J.P.G., M.K.N.K., K.S., and M.R. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Conflicts of Interest: The authors declare no conflict of interest.

Appendix A

Table A1. The accuracy of the emulators developed to estimate the total above-ground dry matter (kg/ha) of rice (WAGT) for different environments in Sri Lanka.

Year	Dry Zone Soil			Intermediate Zone Soil			Wet Zone Soil		
	Sigma sq	CV RMSE	CV RMSSE	Sigma sq	CV RMSE	CV RMSSE	Sigma sq	CV RMSE	CV RMSSE
Year 1	0.13	615.7	1.12	0.17	1272.3	1.04	0.17	1272.3	1.04
Year 2	0.03	233.1	1.11	0.14	927.1	1.06	0.14	927.1	1.06
Year 3	0.10	732.6	1.01	0.28	1736.4	1.04	0.28	1736.4	1.04
Year 4	0.03	150.9	0.92	0.04	371.2	1.11	0.04	371.2	1.11
Year 5	0.05	450.2	1.10	0.24	1594.6	1.06	0.24	1594.6	1.06
Year 6	0.13	998.2	1.11	0.37	1742.5	1.04	0.37	1742.5	1.04
Year 7	0.05	284.1	1.18	0.26	1346.7	1.06	0.26	1346.7	1.06
Year 8	0.03	373.4	1.01	0.18	1056.5	1.09	0.18	1056.5	1.09
Year 9	0.06	438.5	1.08	0.11	919.4	1.03	0.11	919.4	1.03
Year 10	0.06	268.3	1.14	0.21	1358.2	0.96	0.21	1358.2	0.96

Table A2. The accuracy of the emulators developed to estimate the weight of rough rice (kg/ha) of rice (WRR) for different environments in Sri Lanka.

Year	Dry Zone Soil			Intermediate Zone Soil			Wet Zone Soil		
	Sigma sq	CV RMSE	CV RMSSE	Sigma sq	CV RMSE	CV RMSSE	Sigma sq	CV RMSE	CV RMSSE
Year 1	0.14	398.2	1.16	0.21	867.9	1.04	0.14	737.8	1.05
Year 2	0.07	182.5	1.26	0.19	631.4	1.03	0.11	546.2	1.00
Year 3	0.04	309.2	1.01	0.38	777.0	1.05	0.22	845.6	0.98
Year 4	0.12	108.3	0.99	0.11	303.1	1.04	0.09	197.1	1.13
Year 5	0.02	195.8	1.09	0.39	942.7	1.00	0.21	720.8	1.05
Year 6	0.04	383.5	1.04	0.44	752.7	1.02	0.42	1009	1.05
Year 7	0.08	169.0	1.10	0.38	970.3	1.01	0.20	584.3	1.07
Year 8	0.09	197.8	1.19	0.22	553.8	1.04	0.25	524.6	1.06
Year 9	0.12	180.5	1.13	0.26	815.3	1.06	0.11	315.1	1.10
Year 10	0.05	176.4	1.16	0.48	778.1	0.95	0.20	616.9	1.01

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