Computers and Electronics in Agriculture 100 (2014) 1–12

Contents lists available at ScienceDirect

Computers and Electronics in Agriculture

journal homepage: www.elsevier.com/locate/compag

Global sensitivity analysis by means of EFAST and Sobol' methods and calibration of reduced state-variable TOMGRO model using genetic algorithms

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A R T I C L E I N F O

Article history:
Received 4 October 2012
Received in revised form 4 October 2013
Accepted 16 October 2013

Keywords:
TOMGRO
Tomato
EFAST
Sobol
Genetic algorithms
Sensitivity analysis

A B S T R A C T

One common constraint for using crop models for decision making in precise greenhouse crop management is the need for accurate values of model parameters depending on climate conditions, crop varieties, and management. Estimating these parameters from observed data on the crop, using a crop model, is an interesting possibility. Nevertheless, the accuracy of estimations depends on the sensitivity of the model output variables to the parameters. Therefore, this paper proposes the use of the reduced state variable TOMGRO model which describes nodes, leaf area index, total plant weight, total fruit weight, and mature fruit weight as states variables. The objective of this work was to compare EFAST and Sobol' sensitivity analysis methods to determine the most sensitive parameters for TOMGRO model outputs. A former sensitivity analysis showed that 8 parameters were the most sensitive and they were calibrated using genetic algorithms (GAs) to adapt the model to semi-arid weather conditions of Central Mexico. Genetic algorithms are important heuristic search algorithms for optimization problems and have been used to calibrate non-linear models related to control of greenhouse climate conditions. Simulation and analysis of the TOMGRO model showed that the estimations for the state variables are close to the measured data. The model could be adapted for simulating other greenhouse crops by means of sensitivity analysis and calibration.

1. Introduction

There has been an increasing interest in optimal control of greenhouse environments to improve crops production (Bakker et al., 1995; van Straten et al., 2011). Crop growth models can improve the efficiency of a breeding program, as model calculations (sensitivity analysis) enable a quantitative analysis to altering model predictions under a wide range of growing conditions (Boote et al., 2001). Such studies have been published for several crops as cucumber (Marcelis, 1994) and tomato (Heuvelink, 1999; Jones et al., 1999). These explanatory crop growth models are a powerful method to represent and combine knowledge. In contrast to the more common empirical research, explanatory models enable a scientific approach to agricultural problems by incorporating knowledge of underlying processes (Heuvelink et al., 2007). However, the main problem to overcome is to understand the complexities of the crop responses to its environment and management practices as well as the dynamics of the greenhouse environment (Jones et al., 1999). A number of vegetable crop models have been developed for such purposes (Medina-Ruiz et al., 2011; Gary et al., 1998). For example, a number of models have been developed for simulating the dynamic responses of tomato (*Lycopersicon esculentum*) to its environment (Jones et al., 1991; Dayan et al., 1993a,b; de Koning, 1994). These models typically have many state variables like TOMGRO ver. 1.0 has 69 state variables (Jones et al., 1991), and TOMGRO ver. 3.0 has 574 state variables (Kenig and Jones, 1997). Such complexity does not allow knowing how close the solution of the model is to the truly optimal one. If these complex crop models could be simplified by reducing the number of state variables, they would be more useful in optimal control applications. Jones et al. (1999) simplified the TOMGRO model by reducing the number of state variables to five while retaining much of the physiological detail from the comprehensive model. The state variables in the reduced model were selected by lumping fruit into two state variables (total fruit weight, W_F, and mature fruit weight,

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http://dx.doi.org/10.1016/j.compag.2013.10.006

W_M) thereby eliminating age structure and position information. In addition, leaves and stems were lumped together as vegetative tissue, and total plant weight (W) is maintained in the reduced model. Although this reduced tomato model described growth and yield it is not able to simulate growth variables in different tomato varieties and under different management conditions. This means that parameters may have to be estimated for specific management conditions as well as specific varieties (Jones et al., 1999). As the number of parameters increases, the uncertainty of model predictions due to the uncertainty of model parameters becomes more important. Under such conditions, it is important to determine the dominant parameters of the model (Cooman and Schrevens, 2006). Sensitivity analysis is a first step to elucidate the importance of various parameters (Cooman and Schrevens, 2007; Linker et al., 2004; van Straten et al., 1999) in model estimations. Sensitivity analysis evaluates the relative importance of input variables and model parameters on the evolution over time of the model state variables (Saltelli et al., 2000). Global sensitivity analysis apportion outputs uncertainty to the uncertainty of the input factors by taking a sampling approach of probability density functions (PDFs) that provide the inputs for the analysis. Another advantage is that all the parameters vary simultaneously and the sensitivities are calculated over the entire range of each input parameter (Saltelli et al., 2008, 2000; Wallach et al., 2006). Recently, global sensitivity analysis has been applied to open field crop models (Makowski et al., 2006). It has been shown that plant behavior under variable and fluctuating field conditions is affected by adaptation mechanisms that are not operative under controlled conditions. This appeared to apply also to the reduced TOMGRO model parameterized under controlled conditions, which satisfactorily reproduced the results of various experiments conducted under controlled conditions but not under open field conditions because of the higher complexities not explained with only five state variables. Sensitivity analyses on greenhouse crop growth models can be simplified as less state variables are used to describe growing conditions, under greenhouse conditions water and nutrient deficiency could not be treated as well as weeds, pests, and diseases hardly interfere with the growth of crops (Dayan et al., 1993a).

Calibration is another issue of considerable interest which must be performed for adjusting parameters values to obtain a good fit between model outputs and observations (van Straten et al., 2011; Acutis and Confaonieri, 2006). Recently, some research has applied global methods like evolutionary techniques, in particular genetic algorithms (GAs), to perform calibration processes as GA (Guzman-Cruz et al., 2009; Herrero et al., 2007). GA is an optimization and heuristic search technique that uses techniques inspired by evolutionary biology such as inheritance, mutation, selection, and crossover. The selection scheme makes the process towards high performance solutions. A careful selection of genetic algorithm structure and parameters can ensure a good chance of reaching the globally optimal solution after a reasonable number of iterations. Therefore GAs are powerful alternative tools to traditional optimization methods. In former reports of calibration and use of the reduced TOMGRO model extensive sensitivity analysis to variations in climate has been presented only by Cooman and Schrevens (2007). In the presentation and calibration studies of reduced TOMGRO model presented by Jones et al. (1991, 1999), photosynthetically active radiation (PAR) and temperature (T) are varied in an arbitrary range, analyzing the output without apportioning the variations in output to variations in the input. Prior to proper calibration of a mathematical model, it is important to carry out a sensitivity analysis (Van Henten, 2003), which evaluates the relative importance of input variables and model parameters on the evolution over time of the state variables (Saltelli et al., 2000). Then parameter estimation was performed. To achieve an adequate goodness-of-fit of the model, it is necessary to find suitable values for the parameters in the model. In other studies, Bertin (1993) and Dayan et al., 1993a,b, do not include a sensitivity analysis in their calibration and validation of the TOMGRO model. In order to estimate the effect of the factors variation to the model outputs, global approaches estimate the effect of the output of a factor when all the others varying, enabling the identification of interactions in non-linear and/or non-additive models. As a drawback, they are usually computationally expensive to estimate, while local methods can be set to produce system derivatives with a number of model simulations much lower than the number of derivatives to be estimated. The estimation of these local measures can be easily implemented by solving systems of derivatives or taking incremental ratios, but they are informative only if the model is linear or if the range of uncertainty of the input factors is small, the latter condition often ensuring the former (Cariboni et al., 2007). Different techniques have been used to decompose the output variance into the contributions of imputable to each input factor), the most commonly applied are the Extended Fourier Amplitude Sensitivity Test (EFAST) and the Sobol' Method (Saltelli et al., 2008, 2000; Cariboni et al., 2007; Makowski et al., 2006; Sobol', 1990). EFAST decomposes the output variance by means of spectral analysis. The Sobol' method is based on the same decomposition of variance, which is achieved by Monte Carlo methods in place of spectral analysis. Both EFAST and Sobol' methods estimate sensitivity measures which summarize the model behavior. These measures concern the output sensitivity with respect to each factor individually and the total factor sensitivity inclusive of interactions. The most widely used measures, called the main effect or the first-order effect of factor X_i is defined as:

$$S_i = \frac{V_i}{V(Y)}$$

The aim of the current work was to perform a sensitivity analysis on the reduced state-variable TOMGRO model using FAST and Sobol' methods to compare the results in order to select the most sensitive parameters of the model taking into account the different criteria of variance decomposition in both methods. Once the parameters were selected a model calibration was performed using genetic algorithms to compare the results obtained against other reported for the same model.

2. Materials and methods

2.1. Greenhouse conditions and data acquisition

The experiment was carried out under greenhouse conditions from June 2011 to January 2012, using Rafaello tomato variety. Plants were grown hydroponically using volcanic sand as substrate and fertilized with Steiner solution by drip irrigation to provide all nutrients to the plants (Steiner, 1984). Plants were distributed with planting distances of 1.5 m between the rows and 0.5 m between plants within row. Climate conditions were monitored daily and the mean values are shown in Table 1. The climatic variables evaluated were photosynthetic active radiation (PAR, mW m^{-2} s^{-1}), CO_2 concentration (CO, ppm), and temperature (T, °C). Daily measurements of climate variables above mentioned were taken during the whole development of tomato plants with a WatchDog®

Table 1
Values of environmental conditions during the greenhouse experiment.

Climatic variable	Low	Mean	High
Temperature	25	33	40
CO_2 (ppm)	400	550	1100
PAR (μmol/m^2 s)	73.78	221.35	295.14
RH (%)	45	65	85

data logger (Spectrum Technologies, IL, USA), the sampling time was 30 min.

Dry matter was measured each 7 days (from November 4th 2011 to January 22th 2012) from three randomly chosen plants. Plants were dried out during 72 h at 90 °C in an oven. Total dry mass, total fruit dry mass, and total mature fruit dry mass were obtained, the mean of three replications was calculated. Number of nodes and LAI also were recorded each seven days, the leaf area was estimated by means of image processing using a camera based on a CCD sensor MT9M011 (Micron Technology, Boise, ID, USA), the LAI was calculated as the ratio of leaf area/ground area (m^2/m^2).

2.2. Theoretical considerations

The reduced state-variable TOMGRO model is the object of the present research, the five state equations are listed in Table 2. The 29 parameters of the reduced TOMGRO model were included in the sensitivity analysis, parameters which showed small total sensitivity indices indicate a negligible effect of the parameter on the model output and these parameters can be fixed at a nominal value (Factor Fixing Setting). High first-order indices reveal a clearly identifiable influence of the parameter on the model output concerned, and therefore the parameters need to be determined accurately (Factor Priorization Setting). Small first-order indices combined with large interaction indices result in a lack of identification. In practice, the two first rules are commonly used to select the set of parameters to be estimated in a calibration problem. After parameter selection, only 17 parameters were estimated for the experimental conditions (Table 3), the rest were kept the same as in the reduced TOMGRO model (Jones et al., 1999).

2.2.1. Sensitivity analysis

In order to calculate the global sensitivities indices the following procedure was applied (Saltelli et al., 2008):

- **Step 1. Objective specification**. In order to determine which model parameters have a small or large influence on the state variables of the model. Neither input variables nor the initial conditions of the model took part in the sensitivity analysis.
- **Step 2. Factor selection**. Only 17 parameters of the reduced state-variable TOMGRO model were included in the sensitivity analysis.
- **Step 3. Choose of probability density functions (PDFs) for each parameter**. As no further information is available a uniform probability density function was selected for each one of the parameters of the model. Each PDF were selected considering a 10% variation around its nominal value considering information coming from the literature.
- **Step 4. Selection of sensitivity analysis method**. The Extended Fourier Amplitude Sensitivity Test (EFAST) method and the method of Sobol' (Monod et al., 2006) were used, which allows for the calculation of both a first-order sensitivity index and a

Table 2
Description of the reduced TOMGRO model.

Variable	Definition	Equation	Units
N	Number of nodes on mainstem	$\frac{dN}{dt} = N_m \cdot f_N(T)$	Nodes
LAI	Leaf area index	$\frac{d(LAI)}{dt} = \rho \cdot \delta \cdot \lambda(T_d)\frac{\exp[\beta \cdot (N-N_b)]}{1+\exp[\beta \cdot (N-N_b)]} \cdot \frac{dN}{dt}$	m^2/m^2
W	Above ground dry weight	$\frac{dW}{dt} = \frac{dW_F}{dt} + (V_{max} - p_1) \cdot \rho \cdot \frac{dN}{dt}$	g/m^2
W_F	Total fruit dry weight	$\frac{dW_F}{dt} = GR_{net} \cdot \alpha_F \cdot f_F(T_d) \cdot [1 - e^{-\vartheta(N-N_{FF})}] \times g(T_{daytime})$	g/m^2
W_M	Mature fruit dry weight	$\frac{dW_M}{dt} = D_F(T_d) \cdot (W_F - W_M)$	g/m^2

Table 3
Definition and intervals of the TOMGRO parameters used for sensitivity analysis under experimental conditions.

No.	Parameter	Symbol	Units	Nominal value	Upper limit	Lower limit
1	Maximum rate of node appearance	N_m	node d^{-1}	0.495	0.5445	0.4455
2	Maximum leaf area expansion per node	δ	m^2 $node^{-1}$	0.041	0.0975	0.0369
3	Coefficient in expolinear equation	β	$node^{-1}$	0.22	0.242	0.198
4	Projection of linear segment of LAI vs N to horizontal axis	N_b	node	18.5	20.35	16.65
5	Growth efficiency, ratio of biomass to photosynthate available for growth	E	d^{-1}	0.7	0.77	0.63
6	Conversion coefficient of CO_2 to CH_2O	D	g m^{-2} h^{-1}	0.108	0.1188	0.0972
7	CO_2 conductance	τ	μmol m^{-2} s^{-1}	0.0664	0.07304	0.05976
8	Development time from first fruit to first ripe fruit	K	node	0.58	0.638	0.522
9	Light transmission coefficient	m	dimensionless	0.1	0.11	0.09
10	Maintenance respiration coefficient	K_m	g g^{-1} d^{-1}	0.006	0.0066	0.0054
11	Coefficient of biomass partitioning depending on plant development stage	fcN	unitless (0–1 function)	0.85	0.935	0.765
12	Parameter involved in photosynthesis reduction factor	φh	μmolCO_2 m^{-2} s^{-1}	30	33	27
13	Parameter involved in photosynthesis reduction factor	φl	μmolCO_2 m^{-2} s^{-1}	5	5.5	4.5
14	Maximum partitioning of new growth to fruit	α_F	d^{-1}	0.95	1.045	0.855
15	Transition from vegetative development to fruit development	υ	$node^{-1}$	0.24	0.264	0.216
16	Nodes per plant when first fruit appears	N_{FF}	node	14.88	16.368	13.392
17	Radiation utilization efficiency	α	μmol $μmol^{-1}$	0.09	0.099	0.081

Upper and lower values correspond to variations in a 10% respect to the parameter nominal value.

total effect index. The first order sensitivity index (S_i) represents the main effect contribution of each input factor to the variance of the output. The total effect index (S_{Ti}) accounts for the total contribution to the output due to the factor X_i, namely, the first order effect plus higher-order effects due to the interactions among all parameters (López-Cruz et al., 2012a,b).

- **Step 5. Input sample generation**. The SimLab (ver. 3.2) software for sensitivity analysis (SimLab, 2011) was used to generate a sample of size $N = 3000$ by means of EFAST extended method and an $N = 2000$ for Sobol's method to achieve an adequate estimation of sensitivity indices (Saltelli et al., 2004). For EFAST and Sobol' methods the values of sensitivity indices converged within the range of 7000 samples. For most parameters, less than 5000 samples were sufficient to reach a stable value.
- **Step 6. Model evaluation**. A total of 5000 simulations were carried out by the two methods to calculate the five state variables: total fruit weight, W_F, mature fruit weight, W_M, total plant weight, W, number of nodes, N, and leaf area index, LAI. The Runge–Kutta method with variable integration step was used. A relative tolerance of 10^{-8} and absolute tolerance of 10^{-12} was applied to carry out the numerical integration. The model was implemented in MatLab–Simulink environment.
- **Step 7. Analysis of the model outputs**. Both the first-order and the total effect sensitivities indices (S_i and S_{Ti}) were calculated. Bar plots showing both sensitivity indices were generated to evaluate the importance of each parameter. The uncertainty of reduced TOMGRO model state variables was better captured by the normalized sensitivities since they take into account the differences in the ranges of variation of the input factors. The sum of all values is equal to 1 only in the case of additive models and less than 1 in the case of non-additive models (Saltelli et al., 2008).

2.2.2. Calibration of the reduced state-variable TOMGRO model

An appropriate method to perform the calibration is to use a non-linear multivariable optimization function (Tap, 2000), to minimize the sum of square errors (J):

$$J(p) = \sum_{h=1}^{L}\sum_{i=1}^{M}\sum_{j=1}^{N} W_h(\bar{y}_h(t_i,p) - y_{hj}(t_i))^2 \tag{1}$$

$$P^* = argmin J(p)$$

where W_h is the relative weight of each output, $\bar{y}_h(t_i,p)$ is the simulated output, y_h in time t_i, $y_{hj}(t_i)$ is the jth repetition of the measurement y_h in time t_i, L is the number of outputs, M is the number of real measurements (time), N number of repetitions in each real measurement (time), p is the parameter set of calibration and p^* are the parameters that reduce $J(p)$ to a minimum. The weights W_h determine the relative importance of the different outputs in Eq. (1). These were calculated by normalization of the output vector to avoid problems with the units of the state variables. In the present work, minimization of Eq. (1) is reached using evolutionary algorithms (EAs) such as genetic algorithms (GAs).The structure of any EA is the same, differences among evolutionary techniques relies on the kind of selection, mutation, and crossover operators applied to find the optimum value of the parameters to calibrate. In the case of GAs, a string of real values is necessary to represent a candidate solution to a problem (Eiben and Smith, 2003); that is, a vector $(p_1,\ldots,p_s)$ where $p_i \epsilon$ and s is the number of parameters that need to be calibrated. Parent selection is deterministic by means of a tournament (Coello, 2007) which consists in the methodology described by Guzman-Cruz et al. (2009).

The reduced state TOMGRO model contains about 29 parameters. In our case, in order to limit the problems of identifiability,

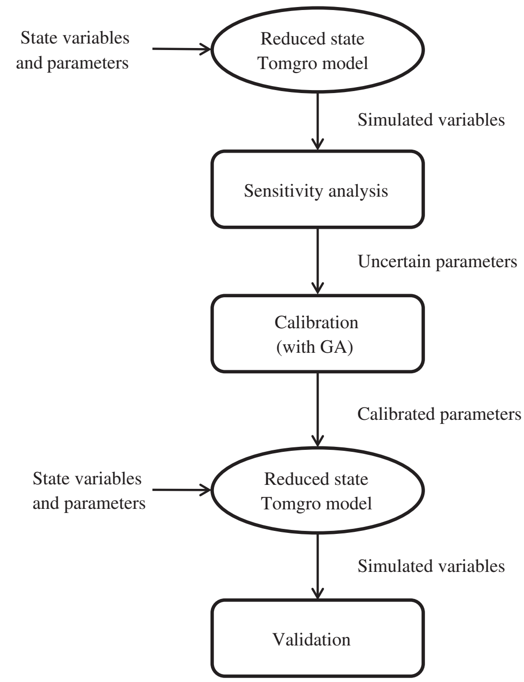

Fig. 1. Diagram of the calibration process of the TOMGRO model (adapted from Guzman-Cruz et al., 2009).

the number of TOMGRO parameters to be estimated has been reduced. First, among the available options for simulating the crop system, the simplest were chosen, after checking that the model was valid for the conditions explored in this publication. Then the tomato system was considered in a similar way to Hernandez-Hernandez et al. (2011) to take as a reference the same parameter nominal values, initial values for TOMGRO parameters were taken from Jones et al. (1999). After the parameter reduction a sensitivity analysis was performed on the 17 resulting TOMGRO parameters. This allowed us to fix those whose effects on the observed variables were negligible, and then according to Varela et al. (2010) for each parameter we computed the values of its effects on the 5 observed variables considered and dropped the parameters for which all these values were less than 10% of the total effects generated by the 17 parameters. We thus restricted the following calibration process to 8 parameters in order to estimate the values which improved the goodness-of-fit of the TOMGRO model to the experimental data of the present work. The process used to calibrate the model is shown in Fig. 1.

2.3. Measuring of goodness-of-fit in greenhouse crop models

The coefficient of determination (R^2) is the measure of correlation between the observations and predictions. Some other important indicators of variances are the percent standard error of the prediction (%SEP), the coefficient of efficiency (E) and the average relative variance (ARV) (Ventura et al., 1995). These estimators are not biased by the variation range of its elements. These are used to determine the capability of the model to explain the total variance of the data. The percent standard error of the prediction is defined as:

$$\%SEP = \frac{100}{\bar{y}k}\sqrt{\frac{\sum_{k=1}^{N}(y_k - \hat{y}_k)^2}{N}} \tag{2}$$

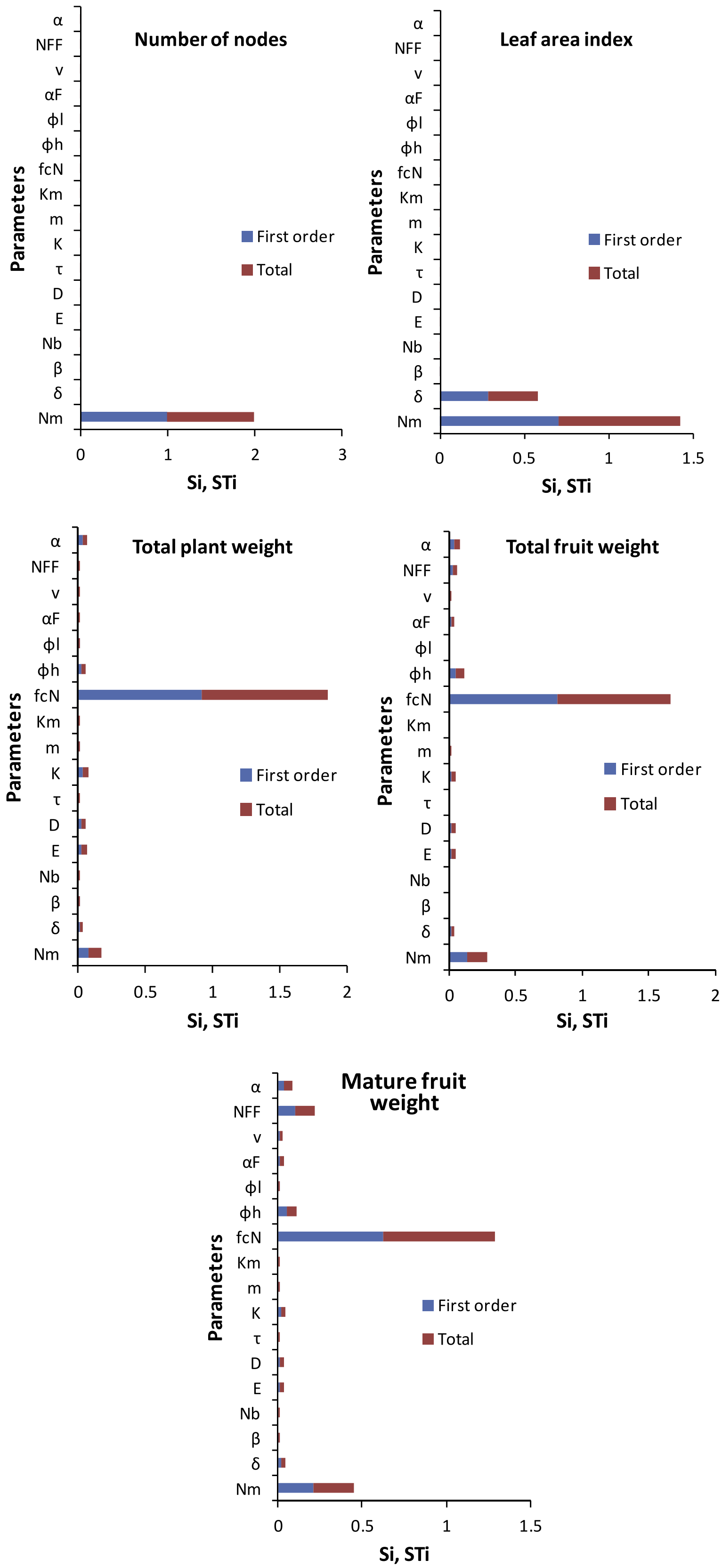

Fig. 2. Global sensitivity indices calculated by EFAST method for TOMGRO state variables.

where y_k is the measured data for each variable; $\hat{y}_k$ is the simulated output of the model; N is the total number of the observations and $\bar{y}_k$ is the mean value of the observed data of the prediction set.

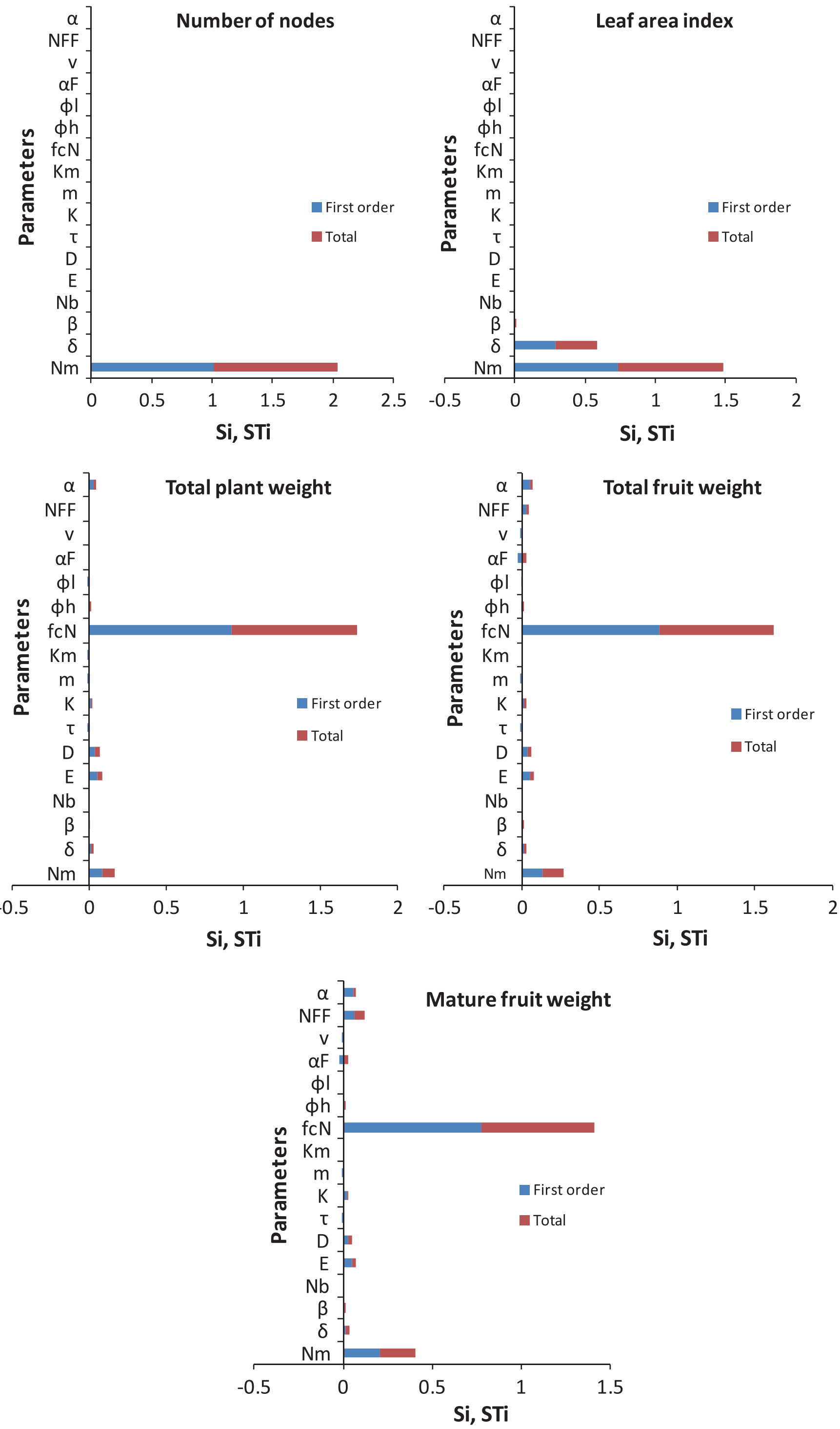

Fig. 3. Global sensitivity indices calculated by Sobol' method for TOMGRO state variables.

The coefficient of the efficiency (E) and the average relative variance (ARV) are expressed by:

$$E = \frac{S_{obs} - S}{S_{obs}}; \quad \mathrm{ARV} = \frac{S}{S_{obs}} \tag{3}$$

$$S_{obs} = \sum_{k=1}^{N} (y_k - \bar{y}_k)^2; \quad S = \sum_{k=1}^{N} (y_k - \hat{y}_k)^2 \tag{4}$$

where S_{obs} is the measure of variability of the observed values from their means and S is the measure of the association between the predicted and observed values. For a perfect match, R^2 and E should be close to 1.0 and the values of %SEP and ARV close to 0. (Rios-Moreno et al., 2006). Also the RMSE was computed to evaluate the errors in the calibration

$$RMSE = \sqrt{\frac{1}{n} \sum_{k=1}^{n} (\hat{y}_k - y_k)^2} \tag{5}$$

$\hat{y}_k$ is the simulated output and y_k is the measured data.

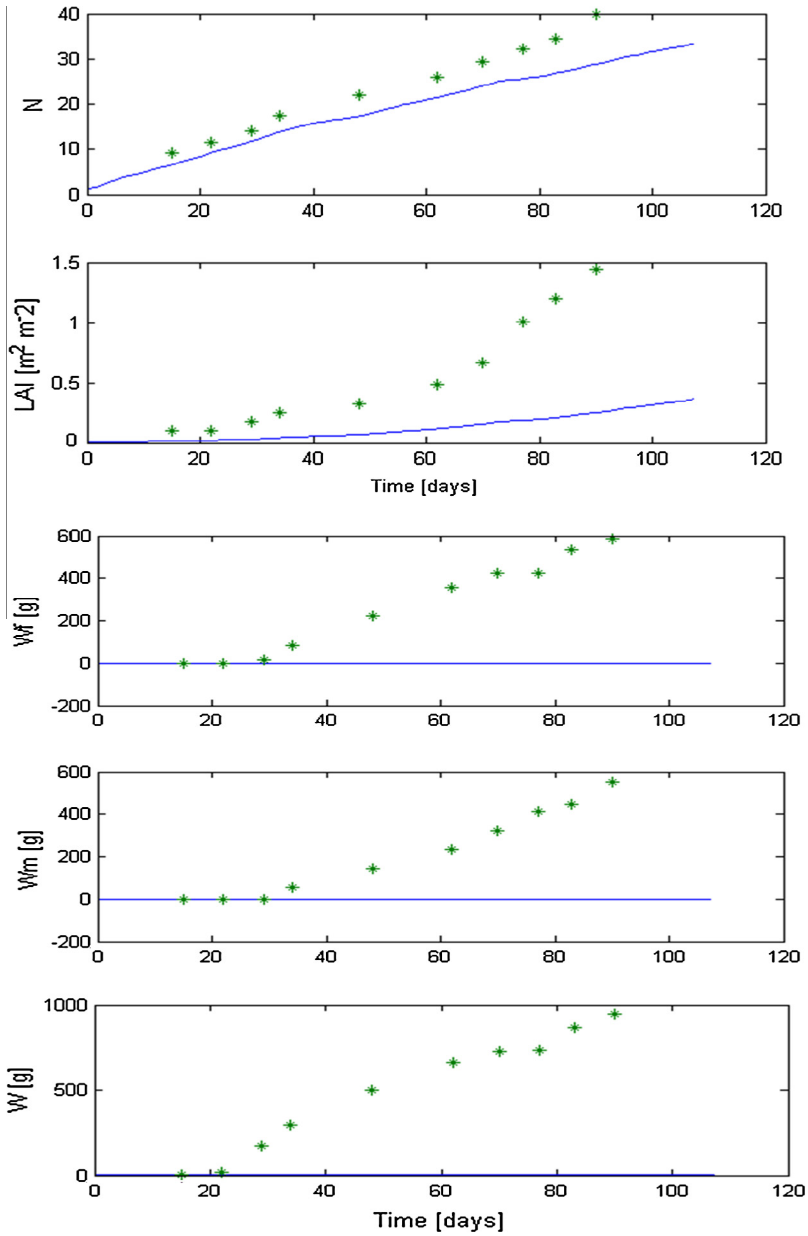

Fig. 4. Measured (dotted line) and simulated (solid line) data before calibration for the 5 state variables in TOMGRO model.

3. Results

3.1. Extended FAST (EFAST) method sensitivity analysis

The sensitivity indices calculated by extended FAST (EFAST) method are shown in Fig. 2 for the five state variables at the end of the growth cycle (105 days). The most important parameters were maximum rate of node appearance (N_m), maximum leaf area expansion per node (δ), ratio of biomass to photosynthate available for growth (E), conversion coefficient of CO_2 to CH_2O (D), development time from first fruit to first ripe fruit (K), coefficient of biomass partitioning depending on plant development stage (fcN), parameter involved in photosynthesis reduction factor (φh), nodes per plant when first fruit appears (N_{FF}), and radiation utilization efficiency (α). For number of nodes, according to the EFAST method (Fig. 2), N_m showed first and total order sensitivity indices of 0.9918 and 1.0, respectively. For leaf area index (LAI) N_m also showed high sensitivity indices (0.7057 and 0.7172, respectively) followed by δ with 0.2841 and 0.2922, respectively. For total plant weight and total fruit weight the most sensitive parameter was fcN with first order and total sensitivity indices between 0.8175 and 0.9178, and between 0.8425 and 0.8175, respectively, followed by N_m. The variable mature fruit weight was more sensitive to fcN (first and total order sensitivity indices of 0.6249 and 0.6689, respectively), followed by N_m, N_{FF}, φ_h, and α.

However, the most important parameters were fcN, N_m, N_{FF}, and E had the larger differences (0.0985, 0.0846, 0.0531, 0.0422, respectively), which means that they explain mostly the interactions among the parameters of the TOMGRO model according to the EFAST method. In order to establish comparison in the sensitivity of the model an analysis with Sobol' method was also performed.

3.2. Sobol' method sensitivity analysis

Fig. 3 shows the first (S_i) and total order (S_{Ti}) sensitivity indices, which are the basic outcome of the Sobol' sensitivity analysis

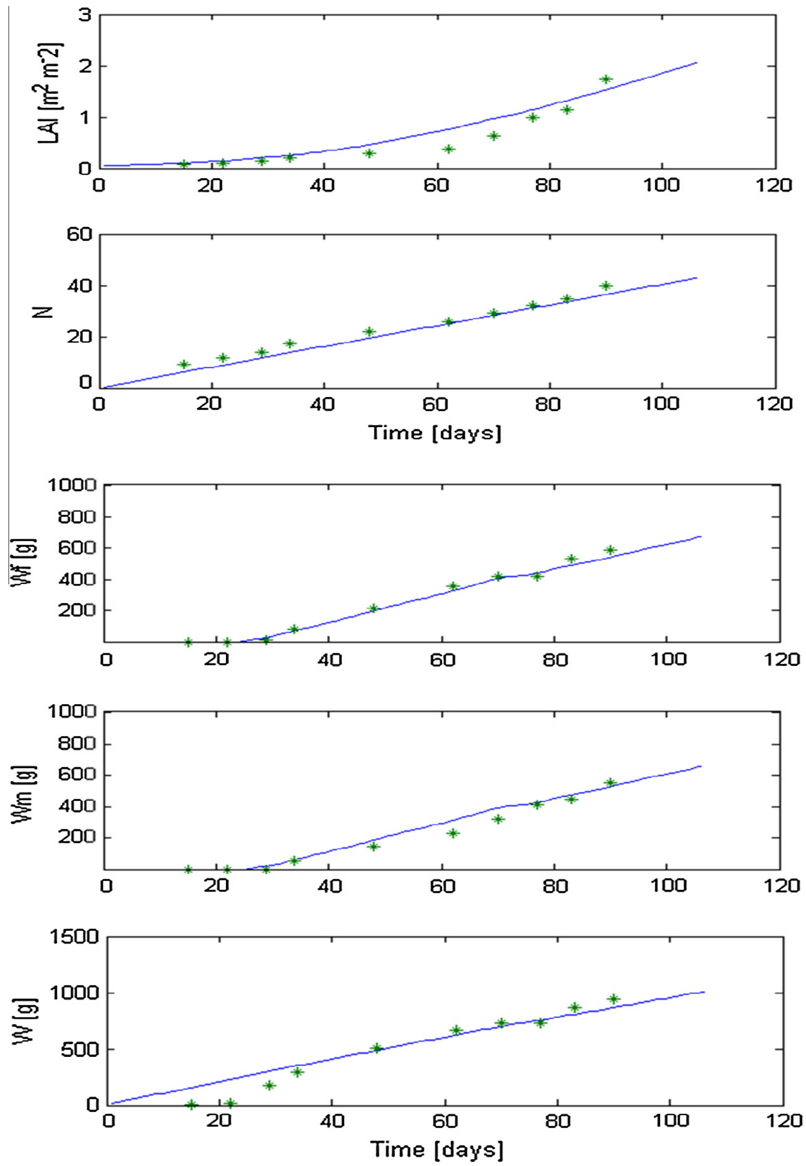

Fig. 5. Measured (dotted line) and simulated (solid line) data after calibration for the 5 state-variables in TOMGRO model.

for all the parameters analyzed. Readers should note that the truncation and Monte Carlo approximations of the integrals required in Sobol's method can lead to small numerical errors (Fieberg and Jenkins, 2005; Sobol', 2001) such as slightly negative values on parameter indices for leaf area index, total plant weight, total fruit weight and mature fruit weight (Fig. 3). In this study these effects were very small and did not impact parameter rankings.

The sensitivity of each state variable to the parameters is shown in Fig. 4. For number of nodes the only parameter which shows sensitivity was N_m. It is clear for LAI that N_m is by far the most sensitive parameter followed by δ (see Table 1 for definition of these parameters). For total plant weight, total fruit weight and mature fruit weight the most important parameter was fcN, the S_i values for this parameter were high which means that this parameter is an important candidate for being calibrated and reduced the uncertainty in model outputs. The same behavior was observed in D, E, N_{FF}, α, and K indicating that these parameters explain much of the variance of the TOMGRO outputs. The most sensitive state variable was mature fruit weight (W_M), a total of eight parameters contribute to the variation in estimations of these variable. Similar results were found with the EFAST method, it showed that total fruit weight (W_F) and mature fruit weight (W_M) were the most sensitive state variables with 8 parameters contributing to its variation. Sensitivity values for parameter K were minor after Sobol' method calibration for W, W_M, and W_F compared to those found with EFAST method. The contribution to uncertainty indicated by Sobol' method was a 50% minor compared to that indicated by EFAST method.

3.3. Calibration of the TOMGRO model by genetic algorithms (GAs)

The results from the EFAST method indicated that only 6 parameters influenced the output of the TOMGRO model being N_m, δ, fcN, N_{FF}, α and K. On the other hand, the Sobol' method pointed out 7 parameters which were N_m, δ, E, D, fcN, N_{FF}, and α. The final set of parameters resulted from combining the results of both methods in order to calibrate them for improving the estimation of the TOMGRO model, the parameters were: N_m, δ, E, D, fcN, N_{FF}, α, and K. The reduction parameter step made during

Table 5
Statistical factors for the five state-variable of the TOMGRO model before and after calibration using GAs for reduced the error between observed and estimated data.

	N		LAI		W		W_F		W_M	
	Before	After	Before	After	Before	After	Before	After	Before	After
%SEP	24.20	10.23	104.51	16.07	120.36	1.20	129.480	9.334	135.12	18.48
ARV	0.330	0.059	1.696	0.105	3.213	0.00032	2.478	0.012	2.210	0.041
E	0.669	0.940	0.696	0.894	2.213	0.999	1.478	0.987	1.210	0.958
R^2	0.895	0.991	0.867	0.964	0.886	0.983	0.646	0.994	0.374	0.976
RMSE	0.59 (104.35%)	2.41 (10.21%)	5.70 (24.16%)	0.149 (25.95%)	592.52 (120.36%)	100.74 (20.46%)	341.22 (129.48%)	24.59 (9.33%)	292.62 (135.12%)	40.02 (18.48%)

validation was in order to improve the performance of the model to the climatic and management conditions considered in this study. It is difficult to accomplish a good adjustment for several state variables simultaneously; the TOMGRO model has 5 state variables which increased the difficulty of the task. So a calibration process is required, this process was performed by means of genetic algorithms (global search method). The Table 2 shows the parameter values before and after calibration, the variation between the original and the calibrated values is due to the original values were used for tomato crops growth in European and North American cold weather conditions. The greenhouse conditions used in this research were very different also the climate control systems performance.

The results before the calibration are shown in Fig. 4. Because of the lack of fit of the simulation to the observed data we decided to perform the sensitivity analysis. It is easy to observe the under estimation of all the variables. The Table 3 shows all the statistical indicators of the goodness-of-fit before and after the calibration in order to compare results. The results for GAs were achieved after 20 runs and the selection was made considering the parameter values which minimized the error between observed and simulated data.

It is clear that the results obtained after the calibration with GAs were better as it was indicated by the statistical factors. After calibration %SEP and ARV were close to 0 as well as E and R^2 were closer to 1.0 for all the state-variables. The R^2 values were closer to 1 after the calibration process for the five state-variables Fig. 5. The statistical factors which showed major improvement were %SEP and ARV with important reductions in all variables, reductions of 58%, 85%, 99%, 92%, and 86% were achieved for N, LAI, W, W_F, and W_M, respectively for the %SEP.

Also important decreases were observed for the ARV in all state-variables remarking the importance of a calibration process. Values for coefficient E ranged between 0.89 and 0.99 after the calibration (Table 3). The Fig. 5 shows the results of the goodness-of-fit of the TOMGRO after the calibration, it is apparent the improvement reached by means of GAs, although LAI is a little overestimated from day 40 to 80 but the statistics showed that it could be considered a good estimation for practical purposes. For number of nodes (N) it was the opposite showing a little underestimation around 10% of the observed data (Fig. 5). The estimated values related to dry weight of plant, total fruits, and mature fruits showed the best fit according with the graphics and the statistical results.

Genetic algorithms showed to be a useful tool for performing calibration tasks, the computational cost was acceptable, using a notebook DELL® XPS L502X equipped with a 2.40 GHz Intel® Core i5 processor and 4.00 Gb RAM memory a run of GAs took about 4 min, the major computational requirements were for sensitivity analysis, each run took about 20 min.

Simulation results using the calibrated values listed in Table 2 were compared against the experimentally measured values of tomato cultivation. Observed maturity dates ranged from 15 to 90 days after transplant, the corresponding simulated values were from 0 to 104 days after transplant. Observed LAI ranged from 0.10 to 1.44 m^2/m^2, the corresponding simulated values were from 0.10 to 1.52 m^2/m^2.

Table 4
Parameter values before and after the calibration process by means of GAs.

Parameter	Original value	Value after calibration
N_m	0.495	0.4039
δ	0.041	0.0875
E	0.70	2.0663
D	0.108	0.3170
fcN	0.85	0.8250
N_{FF}	14.88	4.0116
α	0.056	0.0280
K	0.58	0.3888

The simulated number of nodes did not significantly differ from observed values during the whole days after transplant, with a RMSE = 2.41 nodes (10.21% of the observed mean). The better performance of model estimation could be observed in total fruit weight (W_F) and mature fruit weight (W_M), as it is demonstrated in the high values of E, 0.98 and 0.95, respectively. The RMSE for W_F was 24.59 g (9.33% of the observed mean) and RMSE for W_M was 40.02 g (18.48% of the observed mean). The observed total plant weight was a little overestimated during the first 29 days after transplant, although trough the rest of the days the model estimations adjust very well to the corresponding observed data, this variable showed a RMSE = 100.74 g (20.46% of the observed mean) which was the highest among the dry weights. This overestimation could be due to the parameters could not capture the acclimation effect of tomato plants to the greenhouse environment after the seedling transplant (Besford et al., 1990). In general the model estimated reasonable dry matter weights during the whole growing cycle. After the calibration the RMSE decreased significantly for W, W_F, and W_M being 100.74, 24.59, and 40.02 g respectively, each one below the 20% of the observed mean (Table 3).

4. Results

After the parameter reduction a sensitivity analysis was performed on the 17 resulting TOMGRO parameters. This allowed us to fix those whose effects on the observed variables were negligible, and then according to Varela et al. (2010) for each parameter we computed the values of its effects on the 5 observed variables considered and dropped the parameters for which all these values were less than 10% of the total effects generated by the 17 parameters. We thus restricted the following calibration process to 8 parameters in order to estimate the values which improved the goodness-of-fit of the TOMGRO model to the experimental data of the present work.

4.1. Extended FAST (EFAST) method sensitivity analysis

The sensitivity indices calculated by extended FAST (EFAST) method are shown in Fig. 2 for the five state variables at the end of the growth cycle (105 days). The most important parameters were maximum rate of node appearance (N_m), maximum leaf area expansion per node (δ), ratio of biomass to photosynthate available for growth (E), conversion coefficient of CO_2 to CH_2O (D), coefficient of biomass partitioning depending on plant development stage (fcN), nodes per plant when first fruit appears (N_{FF}), and radiation utilization efficiency (α). For number of nodes, according to the EFAST method (Fig. 2), N_m showed first and total order sensitivity indices of 0.9918 and 1.0, respectively. For leaf area index (LAI) N_m also showed high sensitivity indices (0.7057 and 0.7172, respectively) followed by δ with 0.2841 and 0.2922, respectively. For total plant weight and total fruit weight the most sensitive parameter was fcN with first order and total sensitivity indices between 0.8175 and 0.9178, and between 0.8425 and 0.8175, respectively, followed by N_m. The variable mature fruit weight was more sensitive to fcN (first and total order sensitivity indices of 0.6249 and 0.6689, respectively), followed by N_m, N_{FF}, φ_h, and α.

However, the most important parameters were fcN, N_m, N_{FF}, and E had the larger differences (0.0985, 0.0846, 0.0531, 0.0422, respectively), which means that they explain mostly the interactions among the parameters of the TOMGRO model according to the EFAST method. In order to establish comparison in the sensitivity of the model an analysis with Sobol' method was also performed.

4.2. Sobol' method sensitivity analysis

Fig. 3 shows the first (S_i) and total order (S_{Ti}) sensitivity indices, which are the basic outcome of the Sobol' sensitivity analysis for all the parameters analyzed. Readers should note that the truncation and Monte Carlo approximations of the integrals required in Sobol's method can lead to small numerical errors (Fieberg and Jenkins, 2005; Sobol', 2001) such as slightly negative values on parameter indices for leaf area index, total plant weight, total fruit weight and mature fruit weight (Fig. 3). In this study these effects were very small and did not impact parameter rankings.

The sensitivity of each state variable to the parameters is shown in Fig. 3. For number of nodes the only parameter which shows sensitivity was N_m. It is clear for LAI that N_m is by far the most sensitive parameter followed by δ (see Table 1 for definition of these parameters). For total plant weight, total fruit weight and mature fruit weight the most important parameter was fcN, the S_i values for this parameter were higher compared to S_{Ti} which means that this parameter is an important candidate for being calibrated and reduced the uncertainty in model outputs. The same behavior was observed in N_m, D, E, N_{FF}, and α indicating that these parameters themselves explains much of the variance of the TOMGRO outputs.

4.3. Calibration of the TOMGRO model by genetic algorithms (GAs)

The results from the EFAST method indicated that only 6 parameters influenced the output of the TOMGRO model being N_m, δ, fcN, N_{FF}, α and K. On the other hand, the Sobol' method pointed out 7 parameters which were N_m, δ, E, D, fcN, N_{FF}, and α. The final set of parameters resulted from combining the results of both methods in order to calibrate them for improving the estimation of the TOMGRO model, the parameters were: N_m, δ, E, D, fcN, N_{FF}, α, and K. The reduction parameter step made during validation was in order to improve the performance of the model to the climatic and management conditions considered in this study. It is difficult to accomplish a good adjustment for several state variables simultaneously; the TOMGRO model has 5 state variables which increased the difficulty of the task. So a calibration process is required, this process was performed by means of genetic algorithms (global search method). The Table 2 shows the parameter values before and after calibration, the variation between the original and the calibrated values is due to the original values were used for tomato crops growth in European and North American cold weather conditions. The greenhouse conditions used in this research were very different also the climate control systems performance.

The results before the calibration are shown in Fig. 5. Because of the lack of fit of the simulation to the observed data we decided to perform the sensitivity analysis. It is easy to observe the under estimation of all the variables.

The Table 5 shows all the statistical indicators of the goodness-of-fit before and after the calibration in order to compare results. The results for GAs were achieved after 20 runs and the selection was made considering the parameter values which minimized the error between observed and simulated data.

It is clear that the results obtained after the calibration with GAs were better as it was indicated by the statistical factors. After calibration %SEP and ARV were close to 0 as well as E and R^2 were closer to 1.0 for all the state-variables. The R^2values were closer to 1 after the calibration process for the five state-variables Figs. 5 and 6. The statistical factors which showed major improvement were %SEP and ARV with important reductions in all variables, reductions of 58%, 85%, 99%, 92%, and 86% were achieved for N, LAI, W, W_F, and W_M, respectively for the %SEP.

Also important decreases were observed for the ARV in all state-variables remarking the importance of a calibration process. Values for coefficient E ranged between 0.89 and 0.99 after the calibration (Table 5). The Fig. 5 shows the results of the goodness-of-fit of the TOMGRO after the calibration, it is apparent the improvement reached by means of GAs, although LAI is a little overestimated from day 40 to 80 but the statistics showed that it could be considered a good estimation for practical purposes. For number of nodes (N) it was the opposite showing a little underestimation around 10% of the observed data (Fig. 5). The estimated values related to dry weight of plant, total fruits, and mature fruits showed the best fit according with the graphics and the statistical results.

Genetic algorithms showed to be a useful tool for performing calibration tasks, the computational cost was acceptable, using a notebook DELL® XPS L502X equipped with a 2.40 GHz Intel® Core i5 processor and 4.00 Gb RAM memory a run of GAs took about 4 min, the major computational requirements were for sensitivity analysis, each run took about 20 min.

Simulation results using the calibrated values listed in Table 4 were compared against the experimentally measured values of tomato cultivation. Observed maturity dates ranged from 15 to 90 days after transplant, the corresponding simulated values were from 0 to 104 days after transplant. Observed LAI ranged from 0.10 to 1.44 m^2/m^2, the corresponding simulated values were from 0.10 to 1.52 m^2/m^2.

The simulated number of nodes did not significantly differ from observed values during the whole days after transplant, with a RMSE = 2.41 nodes (10.21% of the observed mean). The better performance of model estimation could be observed in total fruit weight (W_F) and mature fruit weight (W_M), as it is demonstrated in the high values of E, 0.98 and 0.95, respectively. The RMSE for W_F was 24.59 g (9.33% of the observed mean) and RMSE for W_M was 40.02 g (18.48% of the observed mean). The observed total plant weight was a little overestimated during the first 29 days after transplant, although trough the rest of the days the model estimations adjust very well to the corresponding observed data, this variable showed a RMSE = 100.74 g (20.46% of the observed mean) which was the highest among the dry weights. This overestimation could be due to the parameters could not capture the acclimation effect of tomato plants to the greenhouse environment after the seedling transplant (Besford et al., 1990). In general the model estimated reasonable dry matter weights during the whole growing cycle. After the calibration the RMSE decreased significantly for W, W_F, and W_M being 100.74, 24.59, and 40.02 g respectively, each one below the 20% of the observed mean (Table 5).

5. Discussion

The need for ecophysiological models of fruit quality has recently been emphasized (Genard et al., 2007), as models are powerful tools to understand complex system behavior and to point out key-processes and/or key developmental stages involved in the control of complex traits, such as quality. Model application is very often hampered by the fact that appropriate parameterization requires too much effort because complicated experiments under controlled conditions are necessary to establish the required functional relationships (Dayan et al., 1993a,b). In this study two global sensitivity analysis methods were carried out in order to select the most sensitive model parameters to be estimated during calibration process. In tomato horticulture, the Jones et al. (1991) TOMGRO model pioneered the modeling of physiological tomato development by means of basic process calculations as photosynthesis, respiration, node, and leaf development depending on temperature, radiation, and CO_2 concentration as input variables. Since its development on tomato fruit, the generic character of this model has been evaluated on pepper (*Capsicum annum* L.) with only minor modifications (Hernandez-Hernandez et al., 2011), and it was also able to predict the pepper crop development in greenhouse conditions in Mexico with the appropriate sensitivity analysis and calibration. The present work performed a sensitivity analysis and calibration of the reduced state-variable TOMGRO model to be adapted for greenhouse conditions in the Central region of Mexico.

The initial values for TOMGRO parameters were taken from Jones et al. (1991), after the sensitivity analysis 8 parameters were selected do to their high sensitivity indices and after the calibration process, on the whole, the model was able to simulate the growth of tomato. For both methods the sensitivity indices ranged from 0 to 2.5. As result of this analysis, the parameters related to biomass partitioning were very sensitive. Despite a high sensitivity of the model to *fcN* (coefficient of biomass partitioning depending on plant development stage) a constant value could be achieved to simulate the whole range of experimental data. Comparing the goodness-of-fit of the five state-variables, the LAI seemed to be reduced probably due to the inaccurate estimation of the leaf area by means of image processing. Although the sensitivity of β in both methods was negligible for the five state-variables (Figs. 2 and 3), during the factor fixing stage, it was noted that for the LAI slight changes in this parameter led to under- or over-estimations of the LAI during the whole growing cycle. The value found for this parameter by Jones et al. (1991) for different climate conditions was 0.169. In this research the value for this parameter was fixed in 0.158 for the climatic conditions of the Center region in Mexico. Hernandez-Hernandez et al. (2011) found a value of 0.32 for pepper growth simulations similar to those reported by Jones et al. (1999) and Ramirez (2005). Also parameters D and E, related to growth efficiency, showed high sensitivity indices, after calibration the values were 0.31 and 2.06, respectively. These values were higher than those proposed by Jones et al. (1999) (0.108 and 0.70, respectively). Mature fruit appeared to develop faster as indicated by the high value of D and E. The simulated leaf area was slightly higher than observed, this is reflected on the fitting procedure of one of the LAI parameters (δ) which value was twice higher than the proposed by Jones et al. (1999) (Table 2). Temperatures during the whole experiment were high, the value of T_{CRIT} did not show sensitivity to the model but it was increased from 24.0 to 28.0, implying that the variety grown under these conditions was more resistant to high temperatures.

Results for W_F and W_M were described properly by the reduced model after calibration process as shown in Fig. 6 and as indicated by the RMSE values before and after the calibration in Table 3. RMSE values were about 9.33% and 18.48% of the mean observed values. One of the important parameters for fruit production is the stage of development at which time the first fruit starts growing (N_{FF}). The variety used in this research had very large fruit (N_{FF} = 4.01) compared with the varieties studied by Jones et al. (1999).

6. Conclusions

The global sensitivity analysis based on EFAST and Sobol' methods allowed determining the most influential parameters in the TOMGRO model. The EFAST method results showed higher S_{Ti} values which indicate that all the parameters contribute to the model variance in combination. In the other hand, the Sobol' method showed higher S_i values suggesting that this method remarks those parameters to be calibrated in order to reduced output uncertainty. The reduced state-variable TOMGRO model was able to simulate growth and yield of greenhouse tomato growing under semi-arid weather conditions. The calibration produced important information about the importance of climate and management conditions on the performance of the model, LAI goodness-of-fit was the lower among the five state-variables due to the leaf area acquisition methodology which exhibited many variations from sample to sample. The values found for the parameters of the model can be used to simulate other greenhouse crops like pepper when water and nutrients are not limiting, additional work is needed to test this possibility under variable climate conditions in greenhouses and different locations. Further research is needed before we can conclude which method is more reliable when applied to reduced state variable TOMGRO model.

Acknowledgements

The authors wish to acknowledge to FOFI-UAQ 2012 Queretaro and FORDECYT (2012-02) for supporting part of this research. Also M.A. Vazquez-Cruz also thanks to CONACyT for the Ph.D. scholarship support Contract Number 218413, also to Ph.D. Sandra Neli Jimenez Garcia and Ph.D. Luis Miguel Contreras Medina for data acquisition and image processing, and the respective reviewers for their valuable comments and criticisms.

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