Nonlinear Dynamic Lettuce Growth Model: Parameter Selection and Estimation for N-Limited Experiments

Ilya Ioslovich, Marco Ivan Ramirez-Sosa Moran, and Per-Olof Gutman

Abstract— Regulations of European Commission have imposed upper limits of nitrate in lettuce due to possible health hazards for consumers. These nitrate limits create problems for growers in Northern countries. Therefore an effective modeling tool for lettuce growth is necessary. A parameter estimation for a nonlinear three-state model for N-limited lettuce growth in greenhouses is presented in this paper. The variable structural nitrogen concentration and water content are included in the model. The experimental data collected for identification does not allow to readily estimate all parameters of the model, and a recently proposed Dominant Parameter Selection (DPS) method [8], [9] is used to select the set of parameters to be effectively estimated. The calibrated model was perfectly fitted to existing experimental data.

I. INTRODUCTION

High concentrations of nitrate in leafy vegetables such as lettuce constitute a health hazard. Concerned for consumer safety, the EC issued a directive (194/97), defining maximum levels for nitrate in fresh vegetables, including lettuce and spinach. At present, low light levels in winter often make it difficult for growers to meet the required standard. The aim of decreasing winter nitrate levels in crop plants has been the subject of research already for decades. However, a general method, incorporating both accurate control of the internal nitrate concentration and an optimal production management strategy, have not been available.

An useful approach was suggested over a decade ago by [1], showed that the nitrate concentration in lettuce was negatively correlated with the level of soluble carbohydrates. Thus, increased carbohydrate concentrations, associated with stimulated photosynthesis at higher light levels, led to lower nitrate concentrations in lettuce.

This work was generalized in [12] assumed that the pool size of non-structural carbohydrates (including soluble sugars) is determined by the balance between source activity (supply by photosynthesis) and sink activity (demand by maintenance and growth). In view of the strong negative correlation between nitrate and carbohydrate contents, the plant is assumed to posses a regulation mechanism which adjusts the nitrate concentration in its cells to the fluctuating carbohydrate level, in order to meet the turgor requirement.

According to this view, any change in growing conditions which leads to an increase of source activity relative to the sink activity, should result in accumulation of soluble carbohydrates, thus diminishing the need for nitrate as a cellular osmoticum. Hence, the scope for controlling nitrate accumulation in vegetables could be considerably larger than previously thought. Experiments confirm that not only increasing the light level, but also a high atmospheric CO2 concentration, low temperature and growth reduction through a limitation of N-nutrition result in lower levels of nitrate in lettuce. As expected, decreased concentrations of nitrate coincided with increased soluble carbohydrate levels in all cases. A dynamic model, formulated on the basis of this new concept [12], was able to simulate published results of seasonal effects on the nitrate concentration in lettuce [4] with reasonable accuracy. Optimal control policy including reduction of N-supply was presented in [10], [5]. Modeling of crop quality is a relatively new field, in which there is considerable potential for progress. Development of a generic method to accurately control an important quality aspect of greenhouse vegetables, i.e. internal nitrate concentration, constitute a significant contribution to scientific advancement in this field. The EC NICOLET project aimed at further development of the dynamic model of nitrate accumulation in lettuce. Within the scope of the project, the model was studied for different climatic zones of Europe. Independent set of experiments was carried out in UK and described in [2]. It was demonstrated that the model can provide the nutritional decision support for fertilizer. The validation of the model for practical greenhouse conditions has been a very important task. In particular, low N-supply experiments were carried out in the Division of Plant Growth and Development of the Research Station for Floriculture and Glasshouse Vegetables, Aalsmeer, The Netherlands. These experiments revealed several phenomena that were not been successively predicted by the basic model [12]. Among them are essential increase in dry matter content and decrease in Nitrogen in structure (reduced Nitrogen) for severe limitations in Nsupply. To cope with this problem an extension of the model [15] was designed, where the water uptake was assumed to be proportional to N flow into the structure. This model has to be calibrated with existing experimental data, which is the contents of the present paper. We note that the alternative extension of the model was presented in [14], and [11].

A. Model for lettuce growth

The model of the lettuce growth in a greenhouse with N limitation, described in detail in [15], is a multi-input multi-

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I. Ioslovich and P.-O. Gutman are with Faculty of Civil and Environmental Engineering, Technion-Israel Institute of Technology, Haifa 32000, Israel agrilya, peo@tx.technion.ac.il

M.I. Ramirez-Sosa M. is with Departamento de Ingenieria Mecanica y Mecatronica Tecnologico de Monterrey Campus Estado de Mexico, Mexico miramire@itesm.mx

output nonlinear ODE system whose states are the molar mass per $m^2[ground]$ of C in the vacuoles, M_{Cv} , and in the structure of the plant, M_{Cs} , and N in the structure, M_{Ns} .

The inputs are the greenhouse climate variables: light intensity (PAP), I, carbon-dioxide concentration in the air, C_{Ca} , and the air temperature, T.

The measured outputs are fresh matter, F_M , (g/head), dry matter, D_M , (g/head), Nitrate concentration, N_{it} , $(mg[NO_3/kg[FW]])$, and reduced Nitrogen concentration, $N_{red}(g/g[DW])$.

The exchange fluxes of C and N between each two compartments, the atmosphere to the vacuoles and from vacuoles to the structure, (subindexes a, v and s respectively) are represented by the following nonlinear functions:

$$F_{Cav} = p \{I, C_{Ca}\} f \{M_{Ns}\} h_p \{C_{Cv}\},$$

$$F_{Cvs} = \min \left(F_{Cvs}^D, F_{Cvs}^S\right),$$

$$F_{Nvs} = h_N \{C_{Cv}\} r_N F_{Cvs},$$

(1)

where the concentration C_{Cv} is defined below. The demand flux, F_{Cvs}^D , and the real supply flux, F_{Cvs}^S , of C from the vacuole compartment to the structure, are defined as follows:

$$F_{Cvs}^{D} = g \{T\} f \{M_{Ns}\} h_g \{C_{Cv}\},$$

$$F_{Cvs}^{S} = \frac{\beta_N F_{Nnv}^S + \beta_C (F_{Cav} - F_{Cm})}{\lambda \Pi_V + B_C (1 + \theta) + h_N \{C_{Cv}\} r_N (\beta_N + \mu \Pi_V)}$$

The flux F_{Nnv}^S for the non-limited N supply is adjusted to the demand for carbon, and for the N-limited case the rate of growth is adjusted to this flux, as defined in [13]. The flux for maintenance respiration is given by

$$F_{Cm} = f\left\{M_{Ns}\right\} e\left\{T\right\},\,$$

where the basic internal functions of the plant are modeled as: $\mathbf{x} = \mathbf{x}$

$$p\{I, C_{Ca}\} = \frac{\varepsilon I \sigma C_{Ca}}{\varepsilon I \sigma + C_{Ca}},$$

$$e\{T\} = k \exp(c(T - T_*)),$$

$$g\{T\} = me\{T\},$$

$$f\{M_{Ns}\} = 1 - \exp\left(\frac{-aM_{Ns}}{r_N}\right).$$
(2)

For more details on these functions see [13]. The states of the model must hold the algebraic restrictions,

$$\Gamma_{Nv} + \Gamma_{Cv} = 1;$$

$$\Gamma_{Nv} = \frac{\beta_N C_{Nv}}{\Pi_V}, \quad \Gamma_{Cv} = \frac{\beta_C C_{Cv}}{\Pi_V};$$

$$C_{Nv} = \frac{M_{Nv}}{V_V}, \quad C_{Cv} = \frac{M_{Cv}}{V_V};$$

$$V_V = \mu M_{Ns} + \lambda M_{Cs}.$$
(3)

The V_V represents the volume of the plant, and the parameter μ is responsible for the variable water content. It is an important element of the extended model [15]. These algebraic relationships involve some of the parameters, thus those parameters will also have restrictions. Initially all parameters should be strictly positive and for some cases, such as b_p , b_g and b_N must be less than 1 as will be seen later. Thus we

have to use a constrained optimization procedure to estimate the parameters.

Using these notations the differential equations of the model are:

$$\frac{dM_{Cv}}{dt} = F_{Cav} - F_{Cm} - (1 - \theta)F_{Cvs},$$

$$\frac{dM_{Cs}}{dt} = F_{Cvs},$$

$$\frac{dM_{Ns}}{dt} = F_{Nvs} \qquad (4)$$

There are three different inhibition factors used in the model, and related to photosynthesis, growth and the N-uptake. They are defined respectively as:

$$h_{p}\left(\Gamma_{Cv}\right) = \frac{1}{1 + \left(\frac{1 - b_{p}}{1 - \Gamma_{Cv}}\right)^{s_{p}}},$$

$$h_{g}\left(\Gamma_{Cv}\right) = \frac{1}{1 + \left(\frac{b_{g}}{\Gamma_{Cv}}\right)^{s_{g}}},$$

$$h_{N}\left(\Gamma_{Cv}\right) = \frac{1}{1 + \left(\frac{1 - b_{N}}{1 - \Gamma_{Cv}}\right)^{s_{N}}},$$
(5)

Due to the definition of b_g , instead of having a nominal parameter between 0.5 and 1, as in the case of b_p and b_N , we have a positive nominal value less than 0.5, so in order to analyze its sensitivity we use the transformed parameter $\tilde{b}_g = (1 - b_g)$ which is also in the range from 0.5 to 1.

Expressions for the outputs can be found in [13] or [15].

B. Experimental data features

This model has to estimate the measurements of Fresh Matter, F_M (g/head), Dry Matter, D_M (g/head), Nitrate, $N_{it}(mg[NO_3/kg[FW]])$, Nitrogen, N_{red} (g/g[DW]), taken from the experiments carried out in Aalsmeer in 1999, with four treatments: Control (abundant N supply), N supply 12% of the growth demand N, 6% and 0%, respectively, during two periods, July-August (J-A) and September-October (S-O), denoting (2nd line) and enumerating (3rd line) them respectively in (6) and (7) as:

during the first period of July to August and

for the second one from September to October. In the first experiment the four treatments taken together and considered as one measured experiment will be denoted as J - A and enumerated as 9. In the second experiment the four treatments taken together and considered as one measured experiment will be denoted as S - 0 and enumerated as 10. The eight treatments of two experiments will be denoted as J - O and enumerated as 11. Each variable was measured

five times during each one of the experiments 1 - 8: the initial day, the 4th (in the case of S - O on the 3rd), the 7th, the 14th and the 21st days. Some of these treatments were carried out using different addition rates of nutrients from those intended. More details on the experiments can be found in [3].

II. METHODOLOGY OF SENSITIVITY AND CORRELATION ANALYSIS

The objective is to find the optimal set of parameters which minimizes a performance index of the model that is a function of the errors between the measurements and the outputs of the model. For each treatment in the experiments of Aalsmeer we have five sampling instants where the four outputs are measured with different sampling periods, three, four and seven days.

In this case, due to the existence of a limited set of experimental data it is not possible to estimate all the parameters of the model, and it is required to find subset of parameters that can be readily estimated. This will be done using the approach introduced by [9] using the Fisher information matrix to study the sensitivity of the outputs and states of the model on each parameter and the correlation between each pair of them. The condition number of the Fisher matrix related to the complete set of parameters has a very large value, so the matrix is nearly singular, due to the almost zero sensitivity to some parameters in some treatments of periods of the experiments. Another reason is the high correlation between different parameters. With this methodology the set of most sensitive and uncorrelated parameters is selected to be estimated and the computational burden is avoided.

A. Sensitivity and correlation analysis

In order to find the optimal set of parameters (the cost function will be defined later) for the model (4), it is necessary to find the maximal set of parameters to whose variations the outputs of the model are most sensitive, and effects are uncorrelated one to the other. The methodology to be used is the one introduced by [9] which will be shortly described in this section.

Usually in the studies on plant growth models the relative sensitivities are used (see [6], [7]) in order to equalize the data related to different plant ages, and also to eliminate the influence of units. For the outputs of the model, which are nonlinear functions of the three states, which in turn are nonlinear functions of the parameters of the model,

$$\mathbf{Y} = \mathbf{Y} \left\{ M_{Cv}, M_{Cs}, M_{Ns} \right\} =$$

 $\begin{bmatrix} Y_1 \{P, t\} & Y_2 \{P, t\} & Y_3 \{P, t\} & Y_4 \{P, t\} \end{bmatrix}$ (8)

where

$$P = \left[\begin{array}{ccc} p_1 & p_2 & \cdots & p_\ell \end{array} \right], \tag{9}$$

we can find an approximation of the relative sensitivity on each parameter of the model $p_j \forall j = 1, \dots, \ell$. For each output $Y_i \{P, t\}$; i = 1, ..., 4, we define its relative sensitivity to the vector of parameters in the instant t as follows:

$$y^{i}\left\{t\right\} = \frac{P}{Y_{i}\left\{P,t\right\}} \frac{\partial Y_{i}\left\{P,t\right\}}{\partial P}.$$
(10)

To find a numerical approximation of matrix y^i , we first approximate the partial derivatives of the output Y_i with respect to each parameter

$$\frac{\partial Y_i \{P\}}{\partial p_j} \approx \frac{1}{2} \left(\frac{Y_i \{P + \Delta p_j\} - Y_i \{P\}}{\Delta p_j} + \frac{Y_i \{P\} - Y_i \{P - \Delta p_j\}}{\Delta p_j} \right),$$

where

$$P + \Delta p_j = \left[\begin{array}{ccc} p_1 & p_2 & \cdots & (1 + \Delta) p_j & \cdots & p_\ell \end{array} \right].$$

For several treatments (*i.e.* J - A, S - O, and J - O) the matrices y^i have to be vertically concatenated. In such a way, we repeat the process for every parameter in order to construct the matrix y^i of relative sensitivities of the *i*-th output to all parameters. In the matrix y^i the column *j* corresponds to the parameter *j*, and the row *k* corresponds to the measurement instant *k*.

With the relative sensitivity matrix, y^i , we can run the following procedure for the *i*-th output:

- 1) Construct a sensitivity matrix y^i as shown above.
- 2) Find the diagonal values of the Fisher information matrix $F^i = (y^i)^T y^i$, sort the parameters according to the corresponding diagonal value of the Fisher matrix.
- 3) Find the eigenvalues of the Fisher information matrix F^i .
- 4) Select an appropriate maximal threshold condition number α_1 for the Fisher matrix.
- 5) Calculate the normalized sensitivity matrix $y^{iN} = y^i / \sqrt{(y^i)^2}$ and construct the modified Fisher matrix $F^{iN} = (y^{iN})^T y^{iN}$
- 6) The off-diagonal elements of the modified Fisher matrix indicate the pairs of parameters that are correlated. Select the maximum threshold α_2 for the correlation coefficient.
- 7) Select the R' parameters which correspond to the highest diagonal values of the Fisher matrix. Take off each parameter that has correlation coefficient with the previously selected parameters larger than α_2 . Then take the next candidate parameter from the sorted list. Enlarge R' until upper threshold α_1 can be kept.
- 8) Choose these R' parameters and go to step 1 to proceed with the next output.

The algorithms for calculating matrices y^i , and the selection of parameters were implemented in *MATLAB*.

To analyze the four outputs together their sensitivity matrices y^i must be summed with appropriate weighting coefficients.

B. Selection of the parameters to be estimated

In the experiments of Aalsmeer the following variables were measured:

TABLE I OUTPUT MEASUREMENTS

Nitrate	N_{it}	ppm (mg [NO ₃] / kg[FW])
Dry Matter	D_M	g / head
Fresh Matter	F_M	g / head
Reduced N	N_{red}	g / g[DW]

In this section we present the results obtained when applying the sensitivity analysis to each of the corresponding outputs of the model. The parameters to be used as the vector of parameters, P, are: ε , σ (photosynthesis), m, k, θ, c (respiration and growth), a (growth and photosynthesis), $r_N, \lambda, \mu, \beta_N, \beta_C$ (composition), $s_p, s_g, s_N, b_p, b_g, b_N$ (inhibition functions), $M_{Cv0}, M_{Cs0}, M_{Ns0}$ (initial conditions in two experiments). The nominal values are taken as:

TABLE II Nominal Parameters

$\varepsilon = 0.035$	$\sigma = 120.96$	m = 13
k = 0.0216	c = 0.0693	a = 1.7
$r_N = 0.12$	$\lambda = 9.7e - 5$	$\mu = 5e - 3$
$\theta = 0.3$	$\beta_N = 6$	$\beta_C = 0.61$
$s_p = 10$	$s_g = 10$	$s_N = 40$
$b_p = 0.95$	$b_g = 0.2 \left(\widetilde{b}_g = 0.8 \right)$	$b_N = 0.88$
$M_{Cv0}^1 = 0.061$	$M_{Cs0}^1 = 0.251$	$M_{Ns0}^1 = 0.034$
$M_{Cv0}^2 = 0.031$	$M_{Cs0}^2 = 0.255$	$M_{Ns0}^2 = 0.033$

Now we present the sensitivity analysis for each output in the different experiments, which was carried out using a recursive function implemented in *MATLAB* which follows the algorithm presented above.

Using the methodology for each matrix y^i related to the each treatment and each output respectively, with chosen maximum condition number of the resulting Fisher matrix of 8, and a maximum value of correlation between each pair of parameters of 0.95, the sorted uncorrelated parameters are presented in the following tables where the order of the parameters related to the diagonal values of the Fisher matrix (representing the most sensitive to the less sensitive parameters) are given by the numbers in the boxes as: $1, 2, \ldots$ Here the number 1 represents the highest value of the diagonal. In each table the last column contains the condition number of the finally selected Fisher sub-matrix and (in the brackets) the maximum value of correlation between all pairs of parameters in the final obtained set.

C. Sensitivity of the outputs on the parameters

First we consider the matrices y^i separately for each output i = 1, ..., 4. The most sensitive selected parameters for each output are shown in Table III:

TABLE III Most sensitive parameters for each output

	b_p	b_N	\widetilde{b}_g	μ	Cond.
N_{it}		1			1
D_M	1		2		4.3(0.26)
F_M			2	1	2.9(0.09)
N_{red}	1				1

Here one can notice that only one or two parameters can be estimated if only one of the outputs is available. To see the differences between the data obtained from both periods, J - A and S - O, we separate the matrices y^i in two parts, and the results are shown in the Table IV for the first four July-August, (J - A) treatments, and in the Table V for the second four September-October, (S - O) treatments. The results are very similar to the previous analysis.

TABLE IV Most sensitive parameters, J - A

	μ	b_p	b_N	Cond.
N_{it}			1	1
D_M		1		1
F_M	2	1		2.6(0.42)
N_{red}		1		1

TABLE V Most sensitive parameters, S - O

	μ	b_p	b_N	\widetilde{b}_g	Cond.
N_{it}			2	1	2.0(0.28)
D_M		1		2	3.1(0.37)
F_M	1				1
N_{red}		1			1

Thus we can conclude that it is important to include the information given by the all measurements.

When we construct a sensitivity matrix by combining more than one output with a given number of treatments, each single matrix corresponding to each output should be normalized, that is to say, the inverse of the absolute value of the maximum element of each matrix must be multiplied every element in matrix. In this way the final sensitivity matrix will have elements maximum value 1 and the information given by the relative sensitivity matrices is taken into account in the same way for the four outputs. Such multipliers indicate how sensitive an output is to the parameters compared to other outputs, thus these values will be referred as *weights* related to each output and will be used in the performance index for the optimization procedure in the parameter estimation.

Let us consider the hypothetical case that one of the outputs was not measured. Utilizing the eight treatments and the five sampling values, we construct the augmented matrix of sensitivities. Results for the different triplets of outputs are shown in Table VI.

TABLE VI Most sensitive parameters for each triplet of outputs

			b_p	b_N	\widetilde{b}_g	μ	Cond.
N _{it}	D_M	N_{red}	2	1			5.5(0.69)
N _{it}	D_M	F_M	1	2	3	3	5.2(0.67)
N _{it}	F_M	N_{red}	2	1			4.3(0.62)
D_M	F_M	N_{red}	1		3	2	2.64(0.17)

Here the augmented matrix is formed by all sensitivity matrices of the outputs selected. For each treatment, using the enumeration of (6)-(7), we have the following results: In each box, with an integer in it, the integer represents the order number of the parameter from the diagonal of the Fisher matrix, and the condition number of the Fisher matrix, last column, was set to be less than 8. The maximal correlation coefficient is shown in the brackets.

The results for all four outputs and all treatments are shown in the Table VII. Enumeration of the experiments according to the description in Subsection (1. B) above is shown in the first column.

TABLE VII Most sensitive parameters for the four outputs on different treatments and periods.

	ε	β_N	b_p	b_N	\widetilde{b}_g	μ	M_{Ns}^0	r_N	Cond.
1		3			1			2	5.6
2			1						1
3			1			2			1.7
4			1				2		2.4
5	3	2			1				4.0
6			1	3			2		6.2
7			2		1				2.9
8				3	1	2			2.6
9			1	2					5.6
10			1		2	3			1.9
11			1	2	3				6.8

In the last row it can be seen that three parameters can be extracted to fit the four outputs for the experimental data available. The parameter μ could be included if the threshold for the condition number of the Fisher matrix is allowed to be higher than 8.

III. PARAMETER ESTIMATION

The optimal set of parameters for the model depends on the error function used as a criterion and on the nominal values of the parameters. This error function (performance index) was chosen as a quadratic logarithmic function of the error between (weighted) output measurements and estimated outputs by the model, as it is usual for plant growth models.

The methodology given in [9] makes it possible to analyze each measured output, realized treatment, and weather conditions from a nonlinear model, in such a way that enables the selection of those outputs of the real system whose measurement values would give the possibility to extract a higher number of parameters, or even to design experiments for the actual system and estimate the most sensitive parameters for the purposes of optimal control design. In our model we found that all four output measurements should be used to estimate a maximal set of parameters. Combining the sensitivity matrices of the four outputs as in [9], including the eight treatments and the five samplings, the following set of three parameters, using the methodology described before, was found to have the highest sensitivity values with an upper bound of the condition number of the Fisher matrix of 8 and an upper bound for the correlation coefficient of 0.95:

$$P^n = \left[\begin{array}{cc} b_p & b_N & \widetilde{b}_g \end{array} \right]$$

Here the associated Fisher sub-matrix is

$$F = \begin{bmatrix} 12.9 & -7.4 & 1\\ -7.4 & 8.1 & -0.2\\ 1 & -0.2 & 5.9 \end{bmatrix}$$

the condition number is 6.83, and eigenvalues are 2.69, 5.87, 18.35.

The modified Fisher matrix for the correlation values between the parameters is

$$F^N = \begin{bmatrix} 1 & -0.7 & 0.1 \\ -0.7 & 1 & -0.03 \\ 0.1 & -0.03 & 1 \end{bmatrix}.$$

Scaling weights related to each output in each period

$$W_{i} = \frac{1}{\max_{x,y} \left\{ \mathbb{Y}_{i} \left(x, y \right) \right\}}$$

with x, y coordinates of elements of the matrix y^i , were found to be:

W	D_M	F_M	N_{red}	N_{it}
J- A	1/3.1	1/2.0	1/3.5	1/21.2
S-O	1/8.2	1/3.9	1/10.1	1/13.5

These values were used to normalize the sensitivity matrices for the correspondent outputs. The optimal set of estimated parameters, P^o , which minimizes the performance index was found to be:

$$b_p = 0.99$$
 $b_N = 0.965$ $b_g = 0.215$

If the dry matter content, $\frac{D_M}{F_M}$, would have been used instead of the dry matter, D_M , the results are very similar:

$b_p = 0.986$	$b_N = 0.957$	$b_g = 0.22 \left(\widetilde{b}_g = 0 \right)$.78)

For both cases the optimal estimated values of the parameters remain "near" the nominal ones. The fitting of the experimental data by the model is quite perfect as is seen the plots (Fig. 1 and 2).



Fig. 1. Model output and measurements in the experiment of July-August; \Box model, \triangle model (using dry matter content for fitting), * Measurements



Fig. 2. Model outputs and measurements in the experiment of September-October; \Box model, \triangle model (using dry matter content for fitting), * Measurements

IV. CONCLUSIONS

Parameter estimation was performed for a model for lettuce growth in greenhouses under extreme and abundant conditions. The model studied is a modified version of that in [13]. The experimental data used was supplied by the experiments carried out in the Division of Plant Growth and Development of the Research Station for Floriculture and Glasshouse Vegetables, Aalsmeer, The Netherlands, during the periods of July-August and September-October in 1999. The optimal parameter sets were obtained from a specific criterion to be minimized. As motivated in [9], only a subset of the parameters of the model is estimated for the output prediction, and such a subset, selected using the methodology described in [9], is formed by the parameters on which the outputs of the model are most sensitive and each pair of parameters are uncorrelated on a certain level. Perfect fitting was obtained in contrast to the basic variant, thus the modified model is able to fit correctly the plant growth experimental data from two considered treatments and four measured outputs even for the conditions of no supply of N. It is shown that the nominal value of the new parameter μ was chosen in [15] in a reasonable way, thus there was no need for correcting it by estimation.

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