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AN ALGORITHM FOR AUTOMATIC SELECTION AND ESTIMATION OF MODEL PARAMETERS

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Abstract: An algorithm for automatic selection and estimation of model parameters is presented. The algorithm uses a sensitivity matrix based calculation of the parameters effects on the measured outputs and of a linear-independence metric. A predictability degradation index and a parameter correlation degradation index are used as stop criteria and the method is extended to dynamic models and multiple operating points. The applicability of the developed algorithm is illustrated through a hypothetical nonlinear input-output model and through the analysis of data from an experimental isothermal batch bioreactor. The obtained results show the effectiveness of the algorithm.

Keywords: Parameter Estimation, Sensitivity Matrix, Parameter Selection, Principal Component Analysis.

1. INTRODUCTION

Parameter estimation constitutes a key step in the identification and calibration of models. However, often only a subset of the parameters of the model can be estimated, due to limitations in the experimental window and the amount of data. In such a situation, the quality of the estimation is strongly dependent on the selection of the subset of parameters to be estimated. Consequently, a reasonable amount of effort has been made to automating the selection of parameters through the development of adequate criteria and procedures to the execution of this task (Weijers and Vanrolleghem, 1997; Brun *et al.*, 2002; Calvello and Finno, 2004; Ioslovich *et al.*, 2004; Li *et al.*, 2004).

Analysis of sensitivity has proven to be a valuable tool for identifying relevant and uncorrelated parameters. Different strategies based on the use of the sensitivity matrix have been proposed (Weijers and Vanrolleghem, 1997; Li *et al.*, 2004). A particularly systematic and effective identifiability measure method has been proposed by Li *et al.* (2004). In this method the magnitude of each parameter effect on the measured variables is quantified by applying principal-component analysis to a steady-state parameter-output local sensitivity matrix and the determination of the least uncorrelated parameters is accomplished recursively by computing the minimum distance between the sensitivity vector of a candidate parameter and the vector spaces spanned by sensitivity vectors of the parameters already selected for estimation.

Although the method proposed by Li *et al.* (2004) provides an effective ranking of the parameters of a given model, it does not provide criteria to the determination of the optimum number of parameters to be selected for the parameter estimation.

In this work, an algorithm for automatic selection of model parameters based on an extension of the identifiability measure of Li *et al.* (2004) is presented. In this algorithm a predictability degradation index and a parameter correlation degradation index are proposed to be used as stop

criteria. Additionally, the method is extended to dynamic models and multiple operating points.

2. FUNDAMENTALS

The proposed algorithm generates a ranking of the parameters according to their identifiability, measured through the magnitude of their effects on the output variables and a linear-independence metric. The magnitude of the effects of the parameters and the linear-independence metric are calculated from the sensitivity matrix, as proposed by Li *et al.* (2004).

Additionally, a predictability degradation index and a parameter correlation degradation index are defined to be used as stop criteria for the parameter selection algorithm, addressing the question of the number of parameters that should be estimated. The use of the predictability degradation index accounts for the fact the variability of the prediction is expected to increase when the optimum number of selected parameters is overcome. The use of the parameter correlation degradation index is intended to avoid the selection of an unnecessarily high number of parameters, which would increase the correlation between the parameters.

Another important feature in the proposed algorithm is the usage of global sensitivity matrix, which is composed by the information at each experimental point. In this way, the local calculations proposed by Li *et al.* (2004) for the magnitude of the effects of the parameters and the linear-independence metric was easily extended to deal with multiple operating points and dynamic data.

Li *et al.* (2004) have proposed a different dynamic extension procedure, based on a sensitivity matrix to be obtained as the weighted average of the local sensitivity matrices. Although the authors have not implemented this procedure and, consequently, there are not results to be used as basis of comparison, the usage of the global sensitivity matrix is expected to be a more reliable approach. The reason for this statement is that an average sensitivity matrix could lead to loss of information, mainly in problems where the sign of the gains are expected to change.

The definition of the degradation indexes for predictability and parameter correlation as well as the procedure to the calculation of the sensitivity matrix are presented in the next section.

3. AUTOMATIC PARAMETER SELECTION AND ESTIMATION ALGORITHM

The proposed algorithm for automatic selection of model parameters with simultaneous parameter estimation is based on an extension of the identifiability measure of Li *et al.* (2004) and on the proposed predictability degradation index.

For a given set $\{y \in \Re^{ny}, u \in \Re^{nu}\}$ of N experiments (or available process data in N steady-state operating conditions or N dynamic time-points) with r repetitions and a given nonlinear model of the process, the following algorithm is applied to estimate the best possible parameters within a set of $\theta \in \Re^{np}$.

Algorithm SELEST:
1) Evaluate the mean values of y and u for each experiment:

$$\bar{y} = \frac{1}{r}\sum_{k=1}^{r} y_k \in \Re^{ny \cdot N} \quad \text{and} \quad \bar{u} = \frac{1}{r}\sum_{k=1}^{r} u_k \in \Re^{nu \cdot N} \qquad (1)$$

and, if not given, compute the normalized measurement covariance matrix ($V_y \in \Re^{ny \cdot N \times ny \cdot N}$):

$$V_y = \frac{(y - \bar{y} \cdot 1_{1,r})(y - \bar{y} \cdot 1_{1,r})^T}{r-1} \otimes^{-1} \bar{y}\bar{y}^T \qquad (2)$$

where $\otimes^{-1}$ denotes element-by-element division, $1_{1,r}$ denotes a row vector of ones, and $y \in \Re^{ny \cdot N \times r}$.

2) Compute the normalized parameter-output sensitivity matrix, $S \in \Re^{ny \cdot N \times np}$, using an initial estimate of the model parameters, θ_o:

$$S = [S_1^T \; S_2^T \cdots S_N^T]^T \qquad (3)$$

where $S_j = (\Diamond \hat{y}_j)^{-1} \hat{S}_j \, \Diamond \theta_o \in \Re^{ny \times np}$, $\Diamond(\cdot)$ denotes the diagonal matrix of a vector, $\hat{y}_j \in \Re^{ny}$ is the model prediction for the j-th experimental point, using the input mean value $\bar{u}_j$:

$$\begin{aligned} &F(t_j, x, \dot{x}, \bar{u}_j; \theta_o) = 0 \quad , \quad x(0) = \bar{x}_o \\ &\hat{y}_j = H(x, \bar{u}_j; \theta_o) \end{aligned} \qquad (4)$$

and $\hat{S}_j$ is the parameter-output sensitivity matrix evaluated at the j-th point:

$$\hat{S}_j = \frac{\partial H}{\partial x} W_x + \frac{\partial H}{\partial \theta}. \qquad (5)$$

The parameter-state sensitivity matrix, $W_x = \frac{\partial x}{\partial \theta}$, is obtained by solving the following initial-value problem for dynamic processes:

$$\frac{\partial F}{\partial \dot{x}} \dot{W}_x + \frac{\partial F}{\partial x} W_x + \frac{\partial F}{\partial \theta} = 0 \quad , \quad W_x(0) = \frac{\partial x_o}{\partial \theta} \qquad (6)$$

or the linear system:

$$W_x = -\left(\frac{\partial F}{\partial x}\right)^{-1} \frac{\partial F}{\partial \theta} \qquad (7)$$

for steady-state processes.

3) Set m = min {np, $ny \cdot N$} and carry out the singular values decomposition of S left-weighted by the inverse of the normalized standard deviation of the measurements, $\sigma_i = \sqrt{(V_y)_{i,i}}$:

$$(\Diamond\sigma)^{-1}\, S = U\, \Sigma\, V^T \tag{8}$$

or, similarly, carry out the descending-ordered characteristic values decomposition of the Fisher information matrix:

$$F = S^T\, (\Diamond V_y)^{-1}\, S = V\, \Lambda\, V^T, \quad \Lambda = \Sigma^T \Sigma \tag{9}$$

where $\Diamond V_y$ denotes the diagonal matrix composed by the elements of the diagonal of V_y. Then, determine the overall effect of each parameter on the outputs by using the first m principal components (first m column vectors of matrix V, denoted by $V_m \in \Re^{np \times m}$) and the magnitude measure E (Li *et al*., 2004):

$$E = \frac{|V_m|\, \lambda}{\sum_{j=1}^{m} \lambda_j} \quad \in \Re^{np} \tag{10}$$

where $|V_m|$ denotes the matrix with absolute value of the elements of V_m, and λ are the first largest m characteristic values in Λ.

4) Select the highest ranked parameter $p_1 = \{\theta_k \mid E_k = \max_j E_j\}$ and set the number of selected parameters to $n = 1$ and the parameter index set to $\Omega_n = \{k\}$, representing the index set of the best possible parameters to be estimated with the given data set (in descending order).

5) Compute the reduced Fisher information matrix, F_n, regarding to the selected parameters p and the corresponding covariance matrices estimates of the parameters, V_p, and output predictions, $V_{\hat{y}}$:

$$F_n = S_\Omega^T (\Diamond V_y)^{-1} S_\Omega \quad \in \Re^{ny \cdot N \times n} \tag{11}$$

$$V_p = F_n^{-1} \tag{12}$$

$$V_{\hat{y}} = S_\Omega\, V_p\, S_\Omega^T \tag{13}$$

where S_Ω denotes the sub-matrix of S containing only the Ω_n columns. Also, compute the correlation coefficients of these covariance matrices, ρ_p and $\rho_{\hat{y}}$, and the condition number, κ, of F_p:

$$\rho_p = V_p \otimes^{-1} \sqrt{\Diamond V_p\, \Diamond V_p^T} \quad , \quad \overline{\rho}_p = \| \rho_p - I_n \|_{\overline{\infty}} \tag{14}$$

$$\rho_{\hat{y}} = V_{\hat{y}} \otimes^{-1} \sqrt{\Diamond V_{\hat{y}}\, \Diamond V_{\hat{y}}^T} \quad , \quad \overline{\rho}_{\hat{y}} = \| \rho_{\hat{y}} - I_{ny} \|_{\overline{\infty}} \tag{15}$$

$$\kappa = \|F_n\| \cdot \|V_p\| \tag{16}$$

where I_n denotes the identity matrix of size n, and $\| \cdot \|_{\overline{\infty}}$ denotes the highest element of a matrix in absolute value. With this norm definition, $\overline{\rho}_p$ gives the highest correlation among the parameters.

6) Keeping the remaining parameters at the initial estimate θ_o, obtain a new estimate vector $\hat{p}_n$ for the parameters p by least square (or maximum likelihood) parameter estimation for the selected parameters. Also compute the normalized residuals ξ, the predictability degradation index ψ_n, and the parameter correlation degradation index η_n

$$\xi = \frac{1}{r} \sum_{k=1}^{r} [y_k - \hat{y}_k(\hat{p}_n)] \otimes^{-1} y_k \quad \in \Re^{ny \cdot N} \tag{17}$$

$$\psi_n = \overline{\rho}_{\hat{y}} + \| \xi \|_\infty \tag{18}$$

$$\eta_n = \overline{\rho}_p + \delta_{1,n} \tag{19}$$

where $\delta_{i,j}$ is the Kronecker delta. The addition of $\delta_{1,n}$ in Eqn. (19) is necessary to avoid an early stop in step 7 when $n = 2$.

7) Apply the following stop criteria, using a maximum allowed parameter correlation, ρ_{max}:

7.a) If $n > 1$ and ((($\psi_{n-1} < 1$ or ($\eta_{n-1} < \rho_{max}$ and $\eta_n > \rho_{max}$)) and $\psi_{n-1} < \psi_n$) or $\kappa^{-1} < \varepsilon$), then Ω_{n-1} is the solution index set and $\hat{p}_{n-1}$ is the corresponding estimated parameter vector, and terminate the algorithm. ε is the floating-point relative accuracy of the machine.

7.b) If $n = np$, then Ω_n is the solution index set and $\hat{p}_n$ is the corresponding estimated parameter vector, and terminate the algorithm.

8) If $n < m$, then compute the linear-independence metric d_j (Li *et al*., 2004) for each remaining parameter with respect to previously selected parameters:

$$d_j = \sin\left[\cos^{-1}\left(\frac{s_j^T\, V_\Omega\, s_j}{\| s_j \| \cdot \| V_\Omega\, s_j \|} \right) \right], \quad \forall j \notin \Omega_n \tag{20}$$

where $V_\Omega = S_\Omega \left(S_\Omega^T S_\Omega \right)^{-1} S_\Omega^T$. Otherwise, i.e. $n \geq m$, compute the linear-independence metric $d_{q,j}$ for each remaining parameter with respect to all possible (m–1)-tuples Ωq of the previously selected parameters, for

$$1 \leq q \leq \frac{n!}{(m-1)!(n-m+1)!}, \tag{21}$$

where $\Omega q \subset \Omega_n$ and $|\Omega q| = m$–1, using Eqn. (22).

$$d_{q,j} = \sin\left[\cos^{-1}\left(\frac{s_j^T\, V_{\Omega q}\, s_j}{\| s_j \| \cdot \| V_{\Omega q}\, s_j \|} \right) \right], \quad \forall j \notin \Omega_n \tag{22}$$

where $V_{\Omega q} = S_{\Omega q}\left(S_{\Omega q}^T S_{\Omega q}\right)^{-1} S_{\Omega q}^T$. And determine the worst-case metric: $d_j = \min_q d_{q,j}$.

9) Calculate the identifiability index I_j (Li *et al.*, 2004) for each remaining parameter θ_j:

$$I_j = E_j\, d_j \ , \ \forall\, j \notin \Omega_n. \qquad (23)$$

Select the next highest ranked parameter $p_{n+1} = \{\theta_k \mid I_k = \max_j I_j\}$, set the number of selected parameters to $n = n + 1$ and the index set to $\Omega_n = \{\Omega_{n-1}, k\}$, and return to step 5.

It is also possible to add the following diagnostic information in the exit conditions of step 7, evaluated at the stage n-1 (7.a) or n (7.b):

If $\overline{\rho}_{\hat{y}} \geq \rho_{\max}$ and $\overline{\rho}_p < \rho_{\max}$ then the outputs are too much correlated due to possibly high inputs correlation;

If $\overline{\rho}_{\hat{y}} \geq \rho_{\max}$ and $\overline{\rho}_p \geq \rho_{\max}$ then the outputs are too much correlated due to high parameter correlation;

If $\overline{\rho}_p \geq \rho_{\max}$ then the parameters are too much correlated.

The design constant $\rho_{\max}$ of the algorithm is an upper bound for the degree of parameter correlations. This limit is much easier to set than a threshold for the identifiability index I_j, whose value depends much more on experiments than statistic meanings.

4. ILLUSTRATIVE EXAMPLES

In order to illustrate the application of the algorithm SELEST, consider the following hypothetical nonlinear input-output model:

$$\begin{aligned} y_1 &= \theta_1 e^{-\theta_2/u_1} u_2\, u_3 + \theta_3 e^{-\theta_4/u_1} u_2\, u_4 \\ y_2 &= 1 - \theta_1 e^{-\theta_2/u_1} u_2\, u_3 + \theta_5 e^{-\theta_6/u_1} u_3 \\ y_3 &= \theta_7\, u_1 + \theta_8 \left(\theta_1 e^{-\theta_2/u_1} u_2\, u_3 + \theta_5 e^{-\theta_6/u_1} u_3\right) \end{aligned} \qquad (24)$$

with $y \in \Re^3$, $u \in \Re^4$, and $\theta \in \Re^{8+}$. The limited experimental data is composed by $N = 3$ operating points (OP) and $r = 3$ repetitions, shown in Table 1 for three cases. The initial estimate of the model parameters and their exact solution are given in Table 2. The repetitions were generated considering no errors in the inputs, using the exact parameters and adding to the outputs a noise with normal distribution, zero mean, and variance of 5% within 98% of significance level.

In the case 1, the most important input variable, u_1, is kept constant, reducing the estimation capability of the measurements. In the case 3, the last two OPs are correlated. The case 2 is the most favourable data set among the three cases.

Table 1. Experimental data sets for example 1.

	var.	OP_1	OP_2	OP_3
case 1	u_1	0.98	0.98	0.98
	u_2	0.73	0.13	0.43
	u_3	0.23	0.45	0.72
	u_4	0.67	0.47	0.13
	y_1	0.676/0.700/0.710	0.178/0.174/1.175	0.758/0.765/0.762
	y_2	0.623/0.621/0.614	0.933/0.919/0.911	0.332/0.338/0.341
	y_3	7.810/7.508/7.383	6.959/6.903/6.871	9.093/8.889/9.348
case 2	u_1	0.98	0.52	0.75
	u_2	0.73	0.13	0.43
	u_3	0.23	0.45	0.72
	u_4	0.67	0.47	0.13
	y_1	0.676/0.700/0.710	0.058/0.058/0.059	0.537/0.517/0.536
	y_2	0.623/0.621/0.614	0.954/0.969/0.975	0.527/0.545/0.539
	y_3	7.810/7.508/7.383	3.417/3.655/3.532	6.573/6.800/6.761
case 3	u_1	0.98	0.52	0.52
	u_2	0.73	0.13	0.13
	u_3	0.23	0.45	0.45
	u_4	0.67	0.47	0.57
	y_1	0.676/0.700/0.710	0.058/0.058/0.059	0.059/0.059/0.058
	y_2	0.623/0.621/0.614	0.954/0.969/0.975	0.988/0.984/1.002
	y_3	7.810/7.508/7.383	3.417/3.655/3.532	3.489/3.507/3.494

Observing the maximum normalized residuals in Table 2, the reduced-space parameter estimation had similar performance than the full space, showing that the additional parameters would have insignificant improvement in the model predictions. In fact, the index ψ shows the degradation of the predictability for the case 1 when adding the next parameter given by the identifiability index, and a very small improvement in the case 3. In both cases, according to η, the next parameter is highly correlated with the previous selected parameters ($\rho_{\max}$ was set to 0.99). Moreover, the full-space estimations were more sensitive to the initial estimates. The high residuals for the exact parameters are due to the random nature of the noise added to the outputs.

Table 2. Model parameters estimates for example 1. Bold results mean the estimates of the selected parameters in the order shown between parentheses.

par.	exact	θ_o	case 1	case 2	case 3
θ_1	7.65	6.50	6.50	**7.429(5)**	**7.551(5)**
θ_2	1.15	2.40	**0.988(1)**	**1.130(2)**	**1.133(3)**
θ_3	3.89	2.70	2.70	**3.161(3)**	**3.558(4)**
θ_4	1.75	1.50	**1.465(2)**	**1.603(1)**	**1.739(2)**
θ_5	0.23	0.01	**0.116(5)**	**0.136(7)**	**0.086(7)**
θ_6	0.79	0.15	0.15	**0.586(8)**	0.15
θ_7	6.32	4.25	**6.434(3)**	**6.400(4)**	**6.461(1)**
θ_8	3.42	5.50	**3.651(4)**	**3.608(6)**	**3.084(6)**
$\|\xi\|_\infty$	final estimate		0.0259	0.0172	0.0136
	exact		0.0447	0.0330	0.0306
	initial estimate		1.4702	0.8066	0.7774
	full estimate*		0.0261	0.0170	0.0130
ψ	n		1.0206	0.6435	1.0136
	n+1		1.0225	-------	1.0130
η	n		0.7027	0.9983	0.9697
	n+1		1.0000	-------	1.0000

*estimating all np parameters using the exact solution as initial guess.

Applying the diagnostic conditions at exit of step 7 of the algorithm SELEST, the results for the cases 1 and 3 say the outputs are too much correlated due to possibly high inputs correlation, and the parameters are too much correlated in the case 2. Indeed, case 3 was designed with high input correlation in OP_1 and OP_2 and in case 1 all operating points are correlated by the input variable u_1. In case 2, the correlation between θ_1 and θ_2 was the responsible for the high degradation index η_n.

The model parameters were estimated by the least square technique using the Levenberg-Marquardt method with the BFGS (Broyden, Fletcher, Goldfarb, and Shanno) updating scheme for the Hessian matrix (Edgar and Himmelblau, 1988) and relative error tolerance of 10^{-6} for variables and objective function.

Consider now a real example of a multi-route, non-structured kinetic model for microbial growth and substrate consumption of an experimental isothermal batch bioreactor to produce β-galactosidase by *Kluyveromyces marxianus* growing on cheese whey (Longhi *et al.*, 2004). The model is described by a set of five ordinary differential equations:

$$F(t,x,\dot{x},u;\theta) = \dot{x} - f(t,x,u;\theta) = 0 \quad , \quad x(0) = x_o$$
$$y = H(x,u;\theta) \qquad (25)$$

where the states $x \in \Re^5$ are biomass, lactose, ethanol, liquid-phase and gas-phase oxygen concentrations, $u \in \Re$ is the reactor temperature, and $y \in \Re^4$ are x_1, x_2, x_3, and oxygen saturation percentage (pO_2), which is a function of x_4 and u (Longhi *et al.*, 2004). Only one operating condition was used to test the algorithm, at u = 38ºC. The experimental data set is shown in Table 3, and the initial conditions for the state variables are {0.16, 48.90, 0, 0.0075, 1.152}. The model has 12 parameters and their initial estimates are given in Table 4.

Table 3. Experimental data for example 2.

time (h)	y_1 (g/L)	y_2 (g/L)	y_3 (g/L)	y_4 (%)
0	0.16	48.90	0.000	102.5
2	0.19	51.14	0.263	95.5
4	0.30	47.35	0.149	81.9
6	1.68	46.43	0.215	25.5
8	6.59	33.00	2.126	0.8
10	13.09	9.86	11.057	0.2
15	20.42	0.30	6.750	0.1
24	22.74	0.00	0.000	91.2
27	23.11	0.00	0.000	100.6
30	22.65	0.00	0.000	102.9

As shown in Table 4, the tuning of the first ten parameters ranked by the identifiability index got the best predictive capacity from the limited available experimental data. This is also proved in Figure 1, when comparing the prediction of the models adjusted by reduced-space and full-space parameter estimations with the experimental data. The most pronounced difference between the models appears in the dissolved oxygen and ethanol concentrations. In this example ρ_{max} was set to 0.98 and the system of ordinary differential equations was integrated by an implicit BDF method of variable order (Brenan *et al.*, 1989) with relative error tolerance of 10^{-6} and absolute error tolerance of 10^{-8}.

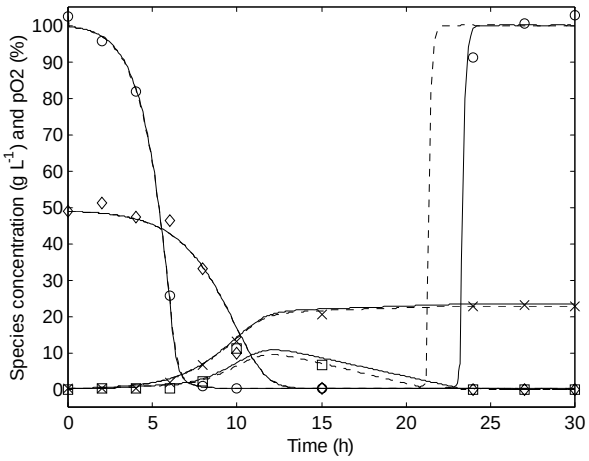

Fig. 1. Experimental data (symbols) for batch culture at 38ºC: (×) biomass concentration (y_1), (◊) substrate concentration (y_2), (□) ethanol concentration (y_3), and (o) dissolved oxygen concentration (y_4); and model predictions with reduced-space (solid line) and full-space (dotted line) parameter estimations.

Table 4. Model parameters estimates for example 2. Bold results mean the estimates of the selected parameters in the order shown between parentheses.

parameters*	θ_o	$\hat{p}$	$\hat{p}$ full
$\theta_1 = \mu_{1max}$	0.60	**0.600(2)**	0.600
$\theta_2 = \mu_{2max}$	0.06	0.06	0.054
$\theta_3 = \mu_{3max}$	0.16	**0.190(10)**	0.206
$\theta_4 = k_1$	20.00	**20.00(4)**	19.953
$\theta_5 = k_{ox1}$	1.00	**1.001(1)**	1.032
$\theta_6 = k_2$	4.26	**4.419(3)**	4.183
$\theta_7 = \phi_{X/S}^{oxid} / Y_{X/S}^{oxid}$	0.63	0.63	0.676
$\theta_8 = \phi_{X/E}^{oxid} / Y_{X/E}^{oxid}$	6.20	**6.257(7)**	6.206
$\theta_9 = 1/Y_{X/S}^{ferm}$	2.44	**2.411(5)**	2.466
$\theta_{10} = 1/Y_{X/S}^{oxid}$	2.63	**2.480(9)**	2.664
$\theta_{11} = \phi_{X/S}^{ferm} / Y_{X/S}^{ferm}$	0.85	**0.935(6)**	0.914
$\theta_{12} = 1/Y_{X/E}^{oxid}$	6.67	**6.257(8)**	6.669
$\|\| \xi \|\|_\infty$	0.1199	0.0787	0.0880
ψ	n	1.0787	1.0880
	n+1	1.0880	-------
η	n	0.9209	0.9860
	n+1	0.9867	-------

* See (Longhi *et al.*, 2004) for parameters definitions.

5. CONCLUSION

An algorithm for automatic selection and estimation of model parameters, based on the identifiability index of Li *et al.* (2004), has been proposed. The predictability and parameter correlation degradation indexes presented good performance as criteria for the determination of the number of parameters that

should be estimated. The usage of the global sensitivity matrix showed to be an adequate strategy to analyze the parameters effects on the outputs when dealing with multiple operating points or dynamic data. The employed examples showed that the algorithm was effective for estimating the best possible subset of parameters within a full set of model parameters, both for steady-state and dynamic models.

REFERENCES

Brenan, K, S. Campbell and L. Petzold (1989). *Numerical solution of initial-value problems in differential-algebraic equations*. Elsevier, New York.

Brun, R., M. Kühni, H. Siegrist, W. Gujer and P. Reichert (2002). Practical identifiability of ASM2d parameters—systematic selection and tuning of parameter subsets. *Water Res.*, **36**, 4113-4127.

Calvello, M. and R. J. Finno (2004). Selecting parameters to optimize in model calibration by inverse analysis. *Comp. & Geotech.*, **31**, 411–425.

Edgar, T.F. and D.M. Himmelblau (1988). *Optimization of Chemical Processes*. McGraw-Hill, New York.

Ioslovich, I., P.-O. Gutman and I. Seginer (2004). Dominant parameter selection in the marginally identifiable case. *Math. Comp. in Simul.*, **65**, 127–136.

Li, R., M.A. Henson and M.J. Kurtz (2004). Selection of Model Parameters for Off-Line Parameter Estimation. *IEEE Transactions on Control Systems Technology*, **12** (3) 402-412.

Longhi, L.G.S., D.J. Luvizetto, L.S. Ferreira, R. Rech, M.A.Z. Ayub and A.R. Secchi (2004). A Growth Kinetic Model of Kluyveromyces marxianus Cultures on Cheese Whey as Substrate. *Journal of Industrial Microbiology*, **31** (1) 35–40.

Weijers, S.R. and P.A. Vanrolleghem (1997). A procedure for selecting best identifiable parameters in calibrating activated sludge model no.1 to full-scale plant data. *Water Sci. Technol.*, **36**, 69-79.