DYNAMIC OPTIMIZATION IN ECOSIMPRO®. APPLICATION TO PARAMETER ESTIMATION AND MODEL VALIDATION

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Abstract

Dynamic optimization techniques are used to solve very interesting problems: fitting of the unknown parameters of a dynamic model, model validation, model based predictive control. In the EcosimPro® modelling and simulation environment, the performance of one optimization solver was analysed, and the problem of model calibration was studied in a systematic way.

Keywords: Dynamic optimization, parameter estimation, sensibility analysis, identifiability.

1. DYNAMIC OPTIMIZATION

There are many applications of optimization in the field of process engineering, ranging from design problems to advanced control techniques as predictive control. Sometimes, as is frequently the case in design problems, the decision variables and the process do not evolve in time but correspond to a determined equilibrium point, so that the optimization decision is a static one. On the contrary, there are other situations in which the variables concerned and the process change in time, so that the problem to solve is a dynamic optimization one.

In a optimization problem with a dynamic system the aim is to minimize a cost function $J(\boldsymbol{u}(t), \boldsymbol{x}(t))$ which depends on the decision variables $\boldsymbol{u}(t)$ and the state variables $\boldsymbol{x}(t)$ of the process, both of them showing an evolution in time. The constraints comprise the differential algebraic system of the model as well as the upper and lower limits of the decision variables and/or others particular to the problem. When the decision variables are real and the relationship among the variables is non linear, the resulting optimization problem is called non-linear programming (NLP).

A general problem with equality and inequality constraints is usually formulated as follows (1):

$$\begin{aligned} &\text{minimize} && J(\boldsymbol{u}, \boldsymbol{x}) \\ &\quad \text{with respect to } \boldsymbol{u} \\ &\text{subject to:} \\ &g_m(\boldsymbol{x},\boldsymbol{u}) \geq 0 && m = 1, 2, \ldots m \\ &h_k(\boldsymbol{x},\boldsymbol{u}) = 0 && k = 1, 2, \ldots k \\ &\boldsymbol{u}_{lower} \leq \boldsymbol{u} \leq \boldsymbol{u}_{upper} \end{aligned} \qquad (1)$$

$$\frac{d\boldsymbol{x}(t)}{dt} = \boldsymbol{f}(\boldsymbol{x}(t), \boldsymbol{u}(t), t)$$
$$\hat{\boldsymbol{y}}(t) = \boldsymbol{g}(\boldsymbol{x}(t), \boldsymbol{u}(t), t)$$

where $\boldsymbol{x}(t)$ are the states of the system, $\hat{\boldsymbol{y}}(t)$ are the model predictions for the measured responses of the system and $\boldsymbol{u}(t)$ is the vector of decision variables.

A dynamic optimization problem can be solved by means of different techniques that try to reformulate it in terms of a NLP one, and that can be classified into two groups: the so called simultaneous methods, where the dynamical part of the constraints is reformulated through the conversion into a set of algebraic equations using either collocation methods or expressions for numerical integration; and the successive methods, based on the integration of the dynamic equations, being these ones the considered in this work.

The decision variables to optimize and the cost function vary depending on the type of dynamic optimization problem considered (parameter estimation, predictive control, etc.). In this work dynamic optimization will be applied to model calibration or parameter estimation. The aim is to find the unknown parameters of a dynamic model so that the responses of the model fit as much as possible the experimental data of the real process. It is a quite challenging question as, in general, there always exist certain parameters that can not be known in a simple way (bibliography, specific experimentation), and that need to be estimated. Thus, the unknown parameters of the model are the decision variables and the cost function evaluates the distance between the model responses for a determined value of these parameters and the experimental data of the process.

1.1 OBJECTIVES

For the parameter estimation by means of dynamic optimization, the model of a very simple process was used. It consists of a tank with an inlet

stream and an outlet stream whose flow of discharge is due to the gravitational force; it is also provided with a stirrer and an electric resistance for heating (Figure 1). The assumptions considered are perfect mixing of the fluid in the tank, constant physical properties and negligible thermal inertia of the vessel. The model is formulated based on the material and energy balances (2 y 3). The measured outputs correspond in this case with the system states: level h, temperature T. The unknown parameters θ_j to estimate are 4: k friction factor of the outlet pipe (θ_1), U_{amb} coefficient of heat losses to the environment (θ_2), A vessel external surface (θ_3), R electric resistance (θ_4). The respective uncertainties in these parameters were supposed to be of ± 25%.

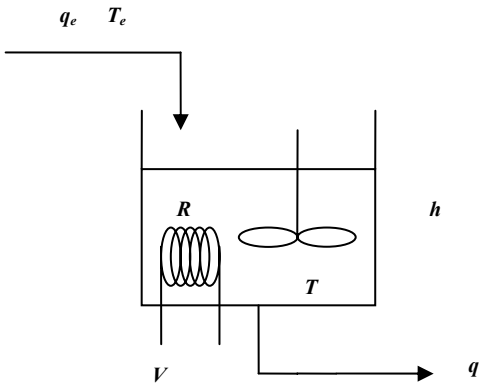

Fig. 1.: Diagram of the tank model

$$A \cdot \frac{dh}{dt} = q_e - k\sqrt{h} \tag{2}$$

$$A \cdot h \cdot \rho \cdot Cp \cdot \frac{dT}{dt} = \tag{3}$$

$$= q_e \cdot \rho \cdot Cp \cdot (T_e - T) + \frac{V^2}{R} - U_{amb} \cdot (T - T_{amb})$$

where q_e and T_e are volume flow and temperature of the inlet stream, ρ and Cp the density and specific heat of the liquid, T_{amb} the temperature of the environment and V the voltage applied to the electric resistance.

The experimental data of the process were obtained in this case through simulation by means of the tank equations, adding a noise signal generated from an ARMA model (auto-regressive moving average).

2. PARAMETER ESTIMATION

Before carrying out the model calibration by means of dynamic optimization techniques, an analysis must be done to determine which among the unknown parameters it is convenient to estimate. For this purpose, a systematic procedure was employed; in the first place the sensibilities of the model responses with respect to the unknown parameters are analysed in order to determine which ones are the most important; in the second place the identifiability of different subsets of parameters (including those parameters that are individually important according to the sensibility analysis) is evaluated; finally, one or several subsets of parameters to estimate are selected.

2.1 SOLUTION BY MEANS OF OPTIMIZATION

The approach to solve a problem of parameter estimation by dynamic optimization considers that for each value of the parameter vector $\boldsymbol{\theta}$ (decision variables) the model yields a prediction of the system response $\hat{\boldsymbol{y}}(\boldsymbol{\theta})$ with a given experiment, that is, for a fixed combination of the manipulated variables.

Real process inputs $\boldsymbol{u}(t)$ and outputs $\boldsymbol{y}(t)$ are sampled over a period of time $t = 1, ..., N$. The same sequence of inputs (manipulated variables) applied to the real process $\boldsymbol{u}(t)$ is applied to the simulated model. For each time t, prediction error $\boldsymbol{e}(t)$ (4) is a measure of model goodness:

$$\boldsymbol{e}(\boldsymbol{\theta}, t) = \hat{\boldsymbol{y}}(\boldsymbol{\theta}, t) - \boldsymbol{y}(t) \tag{4}$$

and the problem to solve is to find the parameter values $\boldsymbol{\theta}$ that minimize prediction errors through an experiment. It can be formulated as an optimization problem according to (5):

$$\min_{\boldsymbol{\theta}} J = \sum_i \sum_{t=1}^{N} \gamma_i \left[e_i(t)\right]^2 = \sum_i \sum_{t=1}^{N} \gamma_i \cdot \left[\hat{y}_i(\boldsymbol{u}, \boldsymbol{\theta}, t) - y_i(t)\right]^2 \tag{5}$$

subject to constraints (6) y (7):

$$\frac{d\boldsymbol{x}(t)}{dt} = \boldsymbol{f}(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{\theta}, t)$$
$$\hat{\boldsymbol{y}}(t) = \boldsymbol{g}(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{\theta}, t) \tag{6}$$

$$\boldsymbol{\theta}_{inferior} \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}_{superior} \tag{7}$$

where J is the objective function that evaluate model fitness to real experimental data for the parameter vector $\boldsymbol{\theta}$, and the sum extends to sampled time t and to each of the measured process outputs i. Although the problem is multiobjective, it is usually better to adjust jointly all the measured outputs in one objective function. Factors γ_i enable to weight in a different way the model fit for each measured output according to the desired accuracy; besides, factors γ_i allow to standardize and make uniform in units the outputs.

So, the objective function is formulated from a weighted least squares criterion. The weights γ_i are usually specified as the reciprocal of the variance due to random noise of the measured outputs $\gamma_i = 1/\sigma_i^2$. In

that way, the subtotals J_i of the objective function corresponding to each output i have comparable values in the optimum, and therefore all the outputs are given the same relative importance in the fit.

According to a formulation (8) equivalent to (5):

$$\min_{\boldsymbol{\theta}} J = \sum_{t=1}^{N} \left[\hat{\boldsymbol{y}}(\boldsymbol{u},\boldsymbol{\theta},t) - \boldsymbol{y}(t)\right]^T \cdot \boldsymbol{Q} \cdot \left[\hat{\boldsymbol{y}}(\boldsymbol{u},\boldsymbol{\theta},t) - \boldsymbol{y}(t)\right] \quad (8)$$

where $\boldsymbol{Q}$ is a diagonal matrix of the aforementioned weights. When the errors in the outputs are not random but correlated, the weight matrix should be equal to the inverse of the variance-covariance matrix of the measured outputs.

Measurement noise and variability due to random disturbances can be characterized from data of the process outputs belonging to an experiment with the manipulated variables at constant value. The variance due to random causes of process output i is estimated according to (9), where $\bar{y}_i$ is the mean value of the output i:

$$\sigma_i^{\,2} = \frac{1}{N-1} \sum_{t=1}^{N} (y_i - \bar{y}_i)^2 \quad (9)$$

Finally, the Fisher Information Matrix (FIM) will be introduced as it will be used later. The FIM is a way of measuring the sensibilities of the model outputs with respect to the parameter vector, and is defined according to (10):

$$\text{FIM} = \left[\sum_{t=1}^{N} \left(\frac{\partial \hat{\boldsymbol{y}}(t)}{\partial \boldsymbol{\theta}}\right)^T \cdot \boldsymbol{Q} \cdot \left(\frac{\partial \hat{\boldsymbol{y}}(t)}{\partial \boldsymbol{\theta}}\right)\right] \quad (10)$$

Although it was not considered in this work, the optimal design of experiments is based on the FIM matrix, since maximizing the FIM –or an associated norm or function– implies maximizing the amount of information obtained from the real system.

2.2 EXPERIMENTAL CAMPAIGN

In the gathering of experimental data of the real process, two sets of data are needed at least, one for the calibration and one for the validation of the model.

Certain considerations must be taken into account in the experiment design stage: choice of a suitable sampling period; appropriate amplitude and frequency of the inputs so as to excite all the fundamental dynamics of the system under study; inputs non correlated were specified; and operating conditions in the range of interest. In Figures 2 and 3 an example of a sequence of inputs applied to the process is shown.

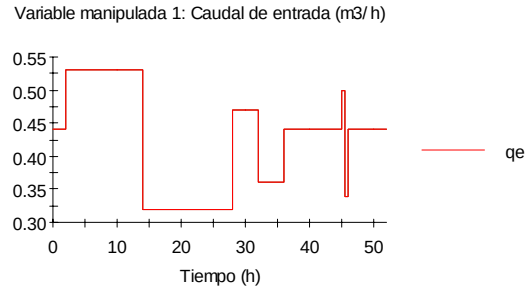

Fig. 2. Sequence in manipulated variable 1

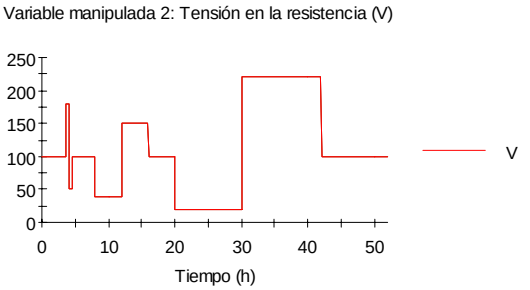

Fig. 3. Sequence in manipulated variable 2

2.3 SENSIBILITY ANALYSIS

Two different sensibilities were studied –relatives, so as to be able to compare–, both depending on the sequence of manipulated variables applied $\boldsymbol{u}(t)$ (that is, on the experiment) and on the point $\boldsymbol{\theta}$ considered in the parametric space:

a) Sensibilities of the objective function to be minimize with respect to the parameter j. The calculation will be usually made by finite differences according to (11):

$$\frac{\partial J}{\partial \theta_j} \approx \theta_{j,inicial} \cdot \frac{J(\theta_j + \Delta\theta_j) - J(\theta_j)}{\Delta\theta_j} \quad (11)$$

although they can also be obtained analytically by numeric integration according to (12):

$$\frac{\partial J}{\partial \theta_j} = 2 \sum_i \sum_{t=1}^{N} \gamma_i \left[\hat{y}_i(\boldsymbol{u}(t),\boldsymbol{\theta},t) - y_i(t)\right] \frac{\partial \hat{y}_i(\boldsymbol{u}(t),\boldsymbol{\theta},t)}{\partial \theta_j} \quad (12)$$

where the partial differentials of the model responses with respect to each parameter $\partial \hat{y}_i / \partial \theta_j$ can be obtained by differentiation with respect to $\boldsymbol{\theta}$ of the equations of the model (6), and taking into account that $\partial \boldsymbol{u} / \partial \boldsymbol{\theta} = 0$ it results (13):

$$\begin{aligned} \frac{d}{dt}\left(\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{\theta}}\right) &= \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{\theta}} + \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{\theta}} \\ \frac{\partial \hat{\boldsymbol{y}}}{\partial \boldsymbol{\theta}} &= \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{x}} \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{\theta}} + \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{\theta}} \end{aligned} \quad (13)$$

being $\partial \boldsymbol{x} / \partial \boldsymbol{\theta}$ the unknown variables. Integrating this system of differential equations (13) jointly with the equations of the model (6), it is possible to obtain the

evolution through time of $\partial \hat{\boldsymbol{y}} / \partial \boldsymbol{\theta}$, and therefore the sensibilities $\partial J / \partial \theta_j$ according to (12).

b) Sensibilities of the responses of the model (outputs) with respect to the parameters according to (14):

$$s_{ij} \approx \frac{\theta_{j,defecto}}{\bar{y}_i} \cdot \frac{\hat{y}_i(t, \theta_j + \Delta\theta_j) - \hat{y}_i(t)}{\Delta\theta_j} \qquad (14)$$

In order to obtain a quantitative measure of the influence of each single parameter j on an output i, the following quadratic mean $\delta_{i,j}^{msqr}$ integrated through time (15) is used:

$$\delta_{i,j}^{msqr} = \sqrt{\frac{1}{N} \sum_{k=1}^{N} s_{ij}^2(k)} \qquad (15)$$

In Figures 4 and 5 the two outputs of the tank model are shown respectively for changes in a single parameter according to the experiment of Figures 2 and 3, so that a first graphical idea of the sensibility can be got.

In Table 1 the numeric values of the sensibilities of the two outputs and the objective function J with respect to the 4 unknown parameters of the tank model are shown as example.

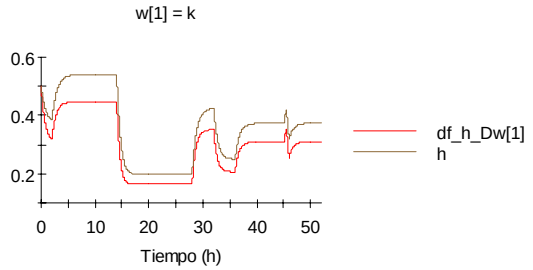

Fig. 4: Sensibility of output 1 vs. θ_1

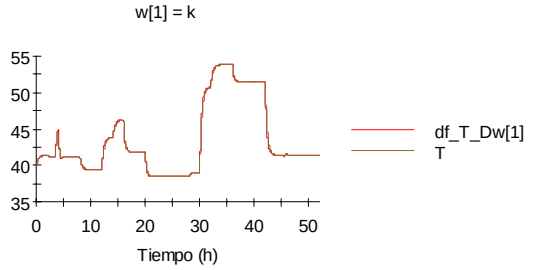

Fig. 5: Sensibility of output 2 vs. θ_1

Table 1

Sensibilities with respect to the 4 parameters to estimate in the tank model

Parameter	$\delta_{1,j}$	$\delta_{2,j}$	$\partial J / \partial \theta_j$
θ_1	1.54	0.04	344
θ_2	0	0.04	-7.3
θ_3	0.06	0.02	-1.1
θ_4	0	0.17	-34

In the analysis carried out [5] it was checked that both sensibilities lead in general to the same conclusions, although with small nuances related to the respective definitions. Sensibilities of the outputs $\delta_{i,j}^{msqr}$ hardly vary from $\boldsymbol{\theta}_{inicial}$ to $\boldsymbol{\theta}^*$, but do not take into account the factors γ_i that weight the different outputs and that are in fact included in the objective function to minimize. Sensibilities of the objective function with respect to each parameter $\partial J / \partial \theta j$ do consider the factors γ_i that weight the different outputs i, however they have the disadvantage of depending too much on the relative position between experimental data and the simulated model for a given $\boldsymbol{\theta}$, and as a result they can lead to mistake when an output fits experimental data much better than other outputs for a given $\boldsymbol{\theta}$.

2.4 IDENTIFIABILITY ANALYSIS

The order of importance of the parameters obtained from the sensibility analysis gives idea of the effect of each parameter –considered alone– on the outputs. Nevertheless, it is also necessary to study the influence of all the parameters together, as it may happen that the effect on an output caused by a change in one parameter is cancelled by another simultaneous change in another parameter. It is then said that there is a certain degree of colinearity in the sensibilities of the outputs with respect to the parameters, which introduces a difficulty in the identification or estimation of the parameter set.

Identifiability is a structural, inherent property that depends on the way the parameters appear in the model, but also on the available measures. The later point can be improved with good experiment design; however, in other cases, nothing can be done. In any case, it is well known that colinearity does not affect negatively the model predictions; but colinearity will determine the accuracy of the parameter estimates obtained.

Two methods were analysed in order to evaluate the identifiability of parameter sets:

a) Brun et al. (2002) method. It is based on the linear dependence of subsets of columns of the sensibility matrix S built from the $\delta_{i,j}^{msqr}$. Brun defines the colinearity index (16):

$$\varphi_K = \frac{1}{\min_{\|\beta\|=1} \left\| \widetilde{S}_K \beta \right\|} = \frac{1}{\sqrt{\lambda_K}} \qquad (16)$$

where $\widetilde{S}_K$ is a submatrix $n \times k$ of $\widetilde{S}$ that contains the columns corresponding to the parameters of the subset K, being n the number of measured outputs and k the number of parameters of the subset K; $\widetilde{S}$ is the sensibility matrix re-scaled or normalized, whose columns are calculated according to (17), and where $\| \delta_j \|$ is the 2-norm of vector δ_j, and λ_K is the smallest eigenvalue of $\widetilde{S}_K{}^T \widetilde{S}_K$.

$$\tilde{\delta}_j = \frac{\delta_j}{\|\delta_j\|} \qquad (17)$$

b) The Fisher Information Matrix (FIM) method. As a measure of the identifiability of the parameters of a model for a given experiment the method uses the condition number for the FIM matrix. This index points out singularity of a matrix, that is, if it is close to a non-invertible matrix. It is calculated as the quotient between the highest and the smallest eigenvalues of the matrix.

High values of the Brun or Fisher indices point out that the corresponding matrix is nearly singular, and as a consequence the parameter subset $\boldsymbol{\theta}$ does not present good identifiability properties. The minimum value of the index is 1 in both methods. Table 2 shows the results for some significant subsets of parameters for the tank model.

It was checked [5] that both methods, in spite of providing similar information, may complement each other in some particular cases. Brun method may lead to colinearity indices abnormally high of two parameters –although the parameters present good identifiability properties according to the model– if both parameters influence the outputs in a similar way (θ_2 θ_4). On the contrary, Fisher method has the advantage that it enables to evaluate more accurately the identifiability according to the model and the experiment considered; however, it may lead to colinearity indices abnormally high of two parameters when the relative sensibilities of the parameters (θ_1 θ_2) differ by orders of magnitude, because in this case the FIM matrix is ill-conditioned. That is the reason why both methods can complement each other.

Table 2.
Identifiability, tank model

Parameter subset	Brun	Fisher
θ_1 θ_2 θ_3 θ_4	∞	1240
θ_1 θ_2	1.01	384
θ_1 θ_3	5.4	434
θ_1 θ_4	1.01	21
θ_2 θ_4	32000	59

Finally, it was analysed [5] how dimensionless standard deviations σ_j calculated from the FIM matrix can alternatively be used to classify parameters in order to select one or more subsets of parameters to estimate, as relative estimation errors (dimensionless standard deviations used in the calculation of confidence intervals) roughly predicted from the FIM matrix for the parameters estimated depend both on the single sensibilities and on the identifiability of the whole subset of parameters.

2.5 ESTIMATION BY OPTIMIZATION

As outlined in point 2, only parameters with high or considerable sensibilities will be estimated, and never those ones with negligible ones. With regard to identifiability, it is of interest that the subset of parameters to estimate has low colinearity. If colinearity is high, there will be lot of combinations of values $\boldsymbol{\theta}^*$ leading to roughly the same J. Nevertheless, a decision can be made to estimate a parameter subset with high colinearity, because usually the estimation of a higher number of parameters improves the fitting to experimental data. However, if the number of parameters to estimate is considerable, it would be natural to select a subset with good identifiability in order to reduce the number of parameters to estimate and in this way make easier the task of the optimization algorithm.

After having selected one or several subsets of parameters, the estimation is carried out by dynamic optimization of a multiobjective function formulated according to a weighted least squares criterion. Experimental data were not filtered since random noise does not influence negatively the optimization and in non-linear models it is not proved that this leads to better estimates.

Table 3
Parameter estimates and confidence intervals, when 4 and 2 param. were estimated

Param.	$\theta_{inicial}$	$\theta^*_{4\ param}$	$\theta^*_{2\ param}$
θ_1	0.72	(0.6195 ± 0.0004)	(0.6195 ± 0.0005)
θ_2	34	(52.4 ± 1.2)	
θ_3	0.47	(0.465 ± 0.007)	
θ_4	7.0	(9.69 ± 0.11)	(11.08 ± 0.09)

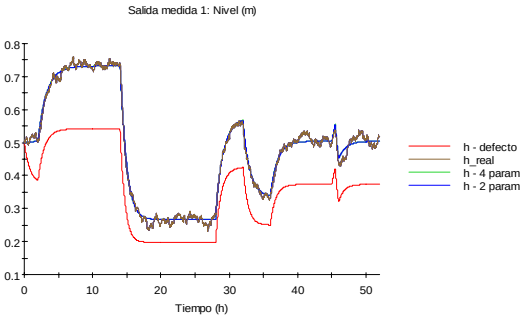

Fig. 6. Measured output 1

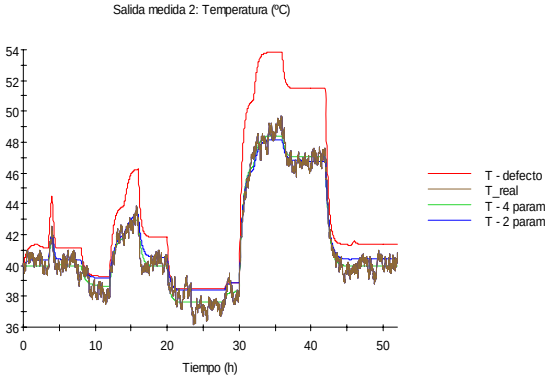

Fig.7. Measured output 2

Parameter estimates (non scaled and with dimensions) obtained when 4 and 2 parameters were estimated for the tank model are shown in Table 3. Figures 6 and 7 represent the difference between model fit to experimental data before and after the parameter estimation, when subsets of 4 and 2 (θ_1 θ_4) parameters were selected.

3. SOLVERS IN THE ECOSIMPRO® ENVIRONMENT

The modelling and simulation environment used, EcosimPro®, provides an object-oriented non-causal approach and is based on powerful symbolic and numerical methods capable of processing complex systems of differential-algebraic equations and discrete events.

As solver for optimization problems formulated in the EcosimPro® environment, a general purpose non linear (NLP) optimization tool was used: a NAG® algorithm based on a sequential quadratic programming SQP method for minimizing. The joint performance of the solver and EcosimPro® was analysed.

The aforementioned SQP algorithm is deterministic. It is fast compared to an heuristic algorithm; however, it does not ensure that the optimum attained is the global and not a local one. Other considerations to be taken into account when optimizing are the scaling of the decision variables to the same order of magnitude, the need to fix lower and upper bounds for the decision variables and the importance of the initial value given to them.

3.1 LIBRERY NAG® ALGORITHM

The convenience of supplying the analytical gradients of the objective function with respect to the decision variables ($\partial J/\partial \theta_j$) to the optimization algorithm was analyzed in order to evaluate the performance of the solver. These gradients are obtained by numerical integration in EcosimPro® according to (12).

Supplying the analytical gradients to the optimization algorithm is of interest because one of the more critical points in the optimum search refers to gradients computation. And it is common in optimization problems where the objective function to minimize is obtained after running a simulation that nearly 90% of the computing time is devoted to model simulation (either to get the objective function value or its gradients with respect to the decision variables), especially when the model is complex; therefore it is important to try to increase the optimum search efficiency. It will be compared to the usual alternative when it is the optimization routine who calculates these gradients by difference quotient by means of objective function evaluations.

The results for different initial conditions and parameter bounds were assessed, according to robustness (final value of J^*), number of iterations of the algorithm and total computing time. On the other hand, it is well known that simulation environment precision has to be greater than that of the solver so that the optimization algorithm produces reliable results when it is necessary to integrate and resolve a system of differential-algebraic equations in order to obtain the objective function. A difference of two orders of magnitude is usually enough. Different tests were also carried out varying computing precisions of the NAG® routine and EcosimPro®.

The conclusion attained is that the optimum found when the analytical gradients numerically integrated in EcosimPro® are given to the optimization routine is never better (neither in value nor in computing time) than the optimum found when it is the routine who evaluates these gradients by difference quotient. So it seems that analytical gradients are expensive to compute and do not lead to increased accuracy as could be expected. So it would be more efficient that the NAG® routine evaluates the objective function gradients with respect to the decision variables by difference quotient, disturbing in a proper extent the decision variables so that the differentials are accurate enough.

4. MODEL VALIDATION

After parameter estimation or model calibration, the resulting model must be validated.

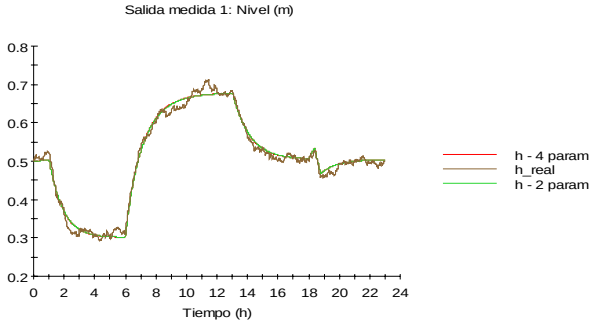

Fig. 8. Validation, output 1

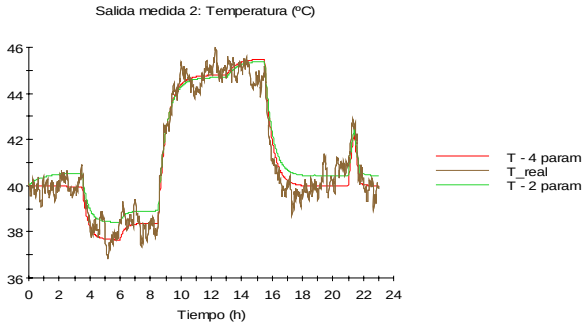

Fig. 9. Validation, output 2

Validation enables to evaluate model credibility according to the specific purpose for which it was formulated. Model reliability is achieved by positive results in a set of tests. Bad results in validation should lead either to another experimental campaign –with other experimental data– or to change the model hypothesis. Different

validation techniques can be used, from graphical comparison with experimental data to statistical tests on the residuals (the difference between the model prediction and the real experimental data). Residuals must be non correlated with the inputs to the process, and should not show noticeable tendencies, that is, should be randomly distributed. If the errors come within acceptable limits, then the model may be deemed capable of explaining the recorded transients.

For a different experiment to the one used in parameter estimation, the model obtained leads to the predicted values that appear in Figures 8 and 9. It can be remarked that the model with 4 estimated parameters fits better to experimental data of the output 2 than the model with 2 estimated parameters, but the difference can be negligible.

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