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A PROCEDURE FOR SELECTING BEST IDENTIFIABLE PARAMETERS IN CALIBRATING ACTIVATED SLUDGE MODEL NO.1 TO FULL-SCALE PLANT DATA

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ABSTRACT

A systematic procedure for selecting identifiable parameter subsets for a given set of measured outputs is proposed. The aim is to only select those parameters which can be estimated uniquely from the dataset used. The proposed procedure consists of first selecting a reduced set of most sensitive parameters by sensitivity analysis and subsequently selecting identifiable parameter subsets using the Fisher information matrix.

For a particular set of outputs obtained from a typical calibration exercise at a carrousel-type nitrogen removal plant, parameter subsets ranging from two to eight parameters were selected by this procedure. The procedure proved successful as the parameter subsets thus selected could be estimated accurately from simulated data without and with noise as well as from real data.

However, the procedure is based on a property which is local in parameter space. Consequently, as an *a priori* assumption on the parameter vales has to be made at the start of the procedure, the selection results might be different from the results which would have been obtained by using the *a posteriori* parameter values. Hence, the sensitivity towards this *a priori* assumption was tested explicitly. For this purpose, the parameter space was sampled according to a Latin hypercube sampling scheme and the selection procedure was applied in all sampling points as if these were *a priori* estimates. From this extensive study it could be concluded that the results of the procedure were not too severely influenced by the *a priori* assumption on the parameter values. Therefore, the proposed procedure appears to be a powerful and practical tool for efficient and reliable model calibration. © 1997 IAWQ. Published by Elsevier Science Ltd

KEYWORDS

Activated sludge; identifiability; mathematical modelling; optimal experimental design; parameter estimation.

INTRODUCTION

In some important applications of the IAWQ Activated Sludge Model No. 1 (as a tool for upgrading existing plants, or as an aid in operation, e.g. for process analysis or model-based control), the model parameters,

influent and sludge characteristics must be fitted to the plant and the conditions in the plant, because some of these show a strong dependency upon plant operation and wastewater composition. This task is referred to as model calibration and it usually requires to perform a combination of input/output measurements on the full-scale plant and additional, lab-scale or pilot-scale experiments, dedicated to assess specific parameters.

In ASM1, several components are distinguished which cannot be measured directly, e.g. readily and slowly biodegradable COD, biomass fractions, etc. The same holds true for the stoichiometric and kinetic parameters. Consequently, these have to be obtained indirectly. In this study the focus will be on the COD fractions and kinetic and stoichiometric parameters, as these are generally considered most problematic. Other parameters, such as parameters defining the plant flowsheet, and initial conditions for the state variables are not considered in this study and are assumed to be either directly measurable or obtainable from separate measurements or experiments.

Despite research efforts by several research groups during the past years, still no established procedure is agreed upon for this model calibration task. As a result, several approaches are being used, which differ in selection of outputs measured and parameters selected for calibration (Weijers *et al.*, 1996). Also in the procedure used for parameter estimation, choices are made by the user (simultaneous or sequential estimation, sequence of estimation). The parameter values obtained may be biased and depend upon the procedure adopted, and thus not have the physical meaning they are thought to have. Besides complicating comparisons of calibration results, application of the calibrated model may also be affected if the parameters obtained are not carefully interpreted. Consequently, it is important to understand the identifiability properties of the model and to develop calibration procedures which reckon with these properties as much as possible.

The focus of this paper is on calibration on the basis of full-scale input/output plant data. It must be known what information is contained in typical output measurements, in order to decide whether and which additional, dedicated experiments are really needed. While efforts have been put into obtaining parameters from well designed pilot tests (Ayesa *et al.*, 1992) this question was not addressed for data obtained during normal operation in full-scale plants, except for Ayesa *et al.* (1995) who applied a reduced order model, however.

The theory section presents two criteria for selecting identifiable parameter subsets and describes the Latin hypercube sampling (LHS) procedure. Then, the proposed procedure for selecting parameter subsets based on this identifiability theory is described, as well as the steps that were taken for testing this procedure by parameter estimations and the LHS-approach. To make this testing realistic, it was performed with a full-scale case study, for which a typical set of output data was available. The results section shows the identifiable parameter subsets obtained by applying the procedure, followed by the estimation results for these selected parameter subsets. These estimations were done by simultaneous estimation of the selected parameters, first using noise-free and noise-corrupted simulated data and then using real data, all for the same set of available outputs. Then the dependency of the parameter subset composition on the *a priori* parameter values is shown on the basis of a Latin hypercube sampling test. Finally, conclusions are drawn.

IDENTIFIABILITY THEORY AND LATIN HYPERCUBE SAMPLING

Criteria for selecting identifiable parameter subsets from data available are described in this section. If least squares parameter estimation is used, the weighted sum J (Eq. 1) of squared errors between model outputs $y(k,\theta)$ and measured outputs $y_p(k)$ with weights R_k is minimised:

$$J = \sum_{k=1}^{N} (y(k,\theta) - y_p(k))^T R_k (y(k,\theta) - y_p(k)). \tag{1}$$

Output sensitivity functions are obtained by linearisation of this functional in the optimal parameter point θ_0:

$$y(t,\theta_o + \delta\theta) = y(t,\theta_o) + \left[\frac{\partial y(t,\theta)}{\partial \theta^T}\right]_{\theta_o} \delta\theta = y(t,\theta_o) + Y_\theta^T(t)\delta\theta \tag{2}$$

with $Y_\theta(t)$ being the output sensitivity functions. Sensitivity functions can be used for selecting parameters (Reichert *et al.*, 1995), as they indicate the relative importance of parameters. For models with many parameters and many outputs, however, it is difficult to reveal all possible dependencies amongst the parameters. This information is summarised in the Fisher information matrix (Mehra, 1974), which can be written as

$$M = \sum_{k=1}^{N} Y_\theta(k) Q_k^{-1} Y_\theta^T(k), \tag{3}$$

here Q_k is the covariance matrix of the measurement noise. Under certain assumptions (no model mismatch, white measurement noise), the inverse of the Fisher matrix provides the lower bound of the parameter error covariance matrix (Söderström and Stoica, 1989):

$$\mathrm{cov}(\theta_o) \geq M^{-1} \tag{4}$$

The above shows that the Fisher matrix relates measurement accuracy, contained in Q_k, and model output parametric sensitivities $Y_\theta(t)$ to parameter estimate accuracy.

Several functions of M can be defined as a measure of the uncertainty on the estimate of θ (Walter and Pronzato, 1990). Two criteria have been applied here, the modified E criterion and the D criterion. The modified E criterion is identical to the condition number, defined as the ratio of the largest to the smallest eigenvalue of M, and thus compares the confidence region's shape with that of a sphere. Although the condition number provides a good indication of identifiability, it was observed that parameter subsets with low condition number were often associated with low traces and determinants, which means that, although parameter estimates may be independent, they may be (very) inaccurate. For this reason, it was decided that the D criterion was to be considered as well. The D criterion is equal to the determinant of M, thus corresponding to the volume of confidence regions (which, by linearisation, become ellipsoids).

For given outputs with measurement error (Q_k) and given number of samples (N), it is the model parametric sensitivities which map the measurement errors onto the parameter error. $Y_\theta(t)$ depends upon the excitation in the input signal, model structure (which are known) and on the (optimal) parameter vector θ_0 (which is not known *a priori* and which is determined by the real output data). Thus with known input signal, model structure, measurement error and number of samples, the identifiability properties depend upon the real output data via the optimal parameter point θ_0.

From the above it is clear that an important limitation of applying the Fisher matrix is that it is a local property, computed in one, optimal, point of parameter space. As the optimal parameter point θ_0 is not known *a priori*, an assumption has to be made, which in general will not coincide with the optimum and thus will not well represent the properties in the optimum. For this reason, the sensitivity towards the *a priori* assumption was investigated by sampling the parameter space according to a Latin hypercube sampling scheme and applying the parameter selection in each of the resulting parameter points, as if these were the *a priori* estimates. Thus, the sensitivity towards the real output data set is also tested. This can be seen as follows. As the optimal parameter point depends upon the output data, a small sensitivity towards the *a priori* assumption implies a small sensitivity towards the real output data set measured.

Latin hypercube sampling includes a stratified sampling of the parameter space which is preferable over random sampling. The scheme is an extension of Latin square sampling and was originally developed by Iman and Conover (1980) to enable sensitivity analysis for time-consuming computer codes through a limited number of simulation runs. For uniform probability distributions on the parameters, the sampling proceeds as follows. A number of samples N_{LHS} is defined. Then the range for each parameter is divided into the same number of N_{LHS} (equally sized) intervals and one observation is made in each interval using random sampling. One observation for the first parameter is then randomly selected, matched with a randomly selected observation on the second parameter and so on for all the parameters. These constitute

sample (parameter point) 1. This procedure is repeated for the remaining parameter observations which exhausts all of the observations and results in a Latin hypercube sample.

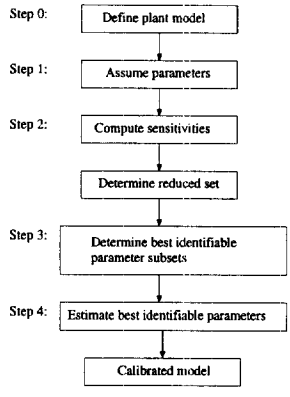

Figure 1. Procedure for selecting best identifiable parameter subsets.

PROPOSED PROCEDURE FOR SELECTING IDENTIFIABLE PARAMETERS

The procedure summarised in Figure 1 is proposed for selecting parameter subsets. The step of the procedure are described in more detail here.

0. Define plant model, input data and initial conditions

It is assumed that the other steps necessary in model calibration have already been taken. These include: (i) obtaining design data such as plant layout and volumes; (ii) obtaining plant input data and operational data as a function of time such as influent flow and concentrations of total COD and Kjeldahl-N, other (internal) flows and loads, temperature, aeration and control loops; also the fractions of soluble Kjeldahl-N and ammonia-N of the total Kjeldahl-N and the COD and Kjeldahl-N concentration of the sludge are assumed to be measured separately; (iii) initial conditions are assumed to be known and obtained either through measurements or through steady state computation; (iv) a set of output measurements such as sludge production, effluent COD, effluent ammonia-N and nitrate-N is available; (v) the model and data are available in computer code. Thus, the next step to be taken is selection of parameters to be estimated and their estimation.

1. Define the set of outputs and an *a priori* parameter set

First, the set of outputs available for estimation is defined. For the analysis, an *a priori* assumption on parameter values has to be made. For example, default values taken from the literature can be applied.

2. Select a reduced set of most sensitive parameters

This step is included to reduce the number of parameters with which the subsequent detailed analysis is done from approx. 25 to a number between 10 and 15 in order to reduce computation time in subsequent steps. Sensitivity coefficients were computed from the mean of the output sensitivity functions:

$$S_{\theta_i}^{y_j} = \frac{\frac{1}{N}\sum_{k=1}^{N}\left|Y_{\theta_i}^{j}(k)\right|}{\frac{1}{N}\sum_{k=1}^{N} y^{j}(k,\theta_0)} \cdot \frac{\delta\theta_i}{\theta_{i0}}. \tag{5}$$

The reduced set was selected according to either of the two following methods: (i) Scale the sensitivity coefficients for each output by the maximal sensitivity coefficient for that output. Select those parameters which show a scaled mean output sensitivity coefficient larger than 0.2 in at least one of the outputs. The idea behind this is to ascertain that at least one parameter will be selected for each output available. (ii) Rank the parameters according to averaged sensitivity coefficients, obtained by averaging over the outputs available:

$$\overline{S^{y}_{\theta_i}} = \frac{1}{N_y} \sum_{j=1}^{N_y} S^{y_j}_{\theta_i} \quad . \tag{6}$$

3. Select those parameter subsets from the reduced set which show highest identifiability
In this step, the Fisher information matrix is computed for all possible subsets of the parameters selected in step 2. This is done for subsets of sizes increasing from 2 to n parameters, yielding the largest possible n (here, n was limited to 8 for reasons indicated in the results section). A ranking is then made of all parameter subsets according to the D as well as to the modified E criterion. For each subset size, the best subset is selected. The listing of best subsets for increasing n provides information on the maximum number of identifiable parameters from the output set. As the number of computations required in this step increases dramatically with the total number of parameters to be evaluated because of combinatorial explosion, the preceding step (obtaining a reduced set) is essential.

4. Estimate selected parameters from real data
If the procedure is successful, then for the parameter subset thus selected unique parameter values are obtained from the real dataset by nonlinear parameter estimation. Other, non-estimated parameters are maintained at their initially assumed values.

TESTING THE SUGGESTED PROCEDURE

To evaluate whether the procedure actually leads to identifiable parameter subsets, the following tests were performed:

1. Estimation from simulated data (i.e. with known 'true' parameter values)
The subsets selected with the above procedure were estimated from simulated data without and with measurement noise added to the outputs. These estimations aimed at i) discriminating between the influence of structural properties and measurement noise and ii) testing whether the identifiability properties from a locally computed Fisher information matrix are sufficiently representative to serve as a basis for selecting identifiable parameter subsets.

2. Estimation from real data
After this, the subsets were estimated from real data, which enables one to i) check whether unique parameter values are obtained despite possibly erroneous *a priori* parameter values and ii) appreciate difficulties encountered in practice, as these data are not as ideal as simulated data, because model mismatch can occur.

3. Assess sensitivity to a priori assumption on the parameter values
Finally, the Latin hypercube sampling was applied as an explicit test for the range of validity of the conclusions with respect to identifiability drawn on the basis of the *a priori* assumed parameter values.

CASE DESCRIPTION

For the study, a wastewater treatment plant of the carrousel type (18.750 m^3) was selected. At this plant, a monitoring campaign has been performed earlier (Weijers *et al.*, 1994). The carrousel was modelled by alternating aerated and non-aerated compartments to achieve nitrogen removal. The two final clarifiers of

the plant were modelled as one static splitter with ideal solids separation. In a measurement campaign of two days the influent and effluent were sampled every two hours.

RESULTS AND DISCUSSION

Procedure results

1. Definition of the set of outputs and *a priori* parameter set

For the analysis of identifiability, a representative set of measured outputs was chosen first. A set consisting of COD, Kjeldahl-N, NH_4 and NO_3 in the effluent and the sludge production was considered representative for typical, standard measurements. Then an *a priori* parameter set was chosen for the analysis. This set consisted of default values for most of the parameters from Henze *et al.* (1987), and the influent COD fractions fS_S, fS_I, fX_S, fX_I and affinity constants K_{OA}, and K_{OH} from an earlier, manual calibration on the same dataset (Weijers *et al.*, 1994). The N fractions were also determined by manual calibration.

2. Selection of a reduced set of most sensitive parameters

A reduced set of most sensitive parameters among the ASM1 kinetic and stoichiometric parameters and COD fractions was selected on the basis of the *a priori* assumption on the parameter values. Output parametric sensitivities were computed, and the selection was done by method (i) described in the procedure section, that is by selecting those parameters which show a time-averaged, scaled sensitivity coefficient larger than 0.2 in at least one of the outputs. The set thus found included Y_H, μ_H, b_H, Y_A, μ_A, K_S, K_{OA}, η_g, fS_I, fX_I and fX_{BH}. In this particular case, the aerated volume fraction also appeared to be very important, which is an artefact introduced by the flowsheet used. For this reason in the sequel this parameter will not be considered for estimation. With this reduced set, the following step could be carried out.

3. Identifiable parameter subsets selection

For the reduced parameter set, for all parameter subset combinations containing 2 to 8 parameters, the Fisher matrix was computed. For this computation, the output error covariance matrix Q_k was assumed diagonal and constant over the samples, and for each output the error was assumed to be proportional with the mean value over the samples for that output. An additional scaling of the sensitivity functions by the *a priori* parameter values was applied. The subsets were subsequently ranked according to the determinant (D criterion) and condition number (Modified E criterion) (results not shown). The subsets yielding the highest determinant, respectively the lowest condition number were selected. These results indicated that it was best to use a combined criterion, and from the parameter subsets with the best determinants that subset was chosen which had a significantly lower condition number than surrounding sets. Table 1 was produced using this heuristic procedure.

Table 1. Parameter subsets selected with combined criterion

Subset size	Determinant	Cond. Number	Parameter subset
2	$1.44\ 10^4$	4.795	fX_I, $\mu_A 20$
3	$11.0\ 10^4$	35.1	fX_I, fS_I, $\mu_A 20$
4	$50.2\ 10^4$	110	$b_H 20$, fX_I, fS_I, $\mu_A 20$
5	$104.1\ 10^4$	295	$b_H 20$, fX_I, fS_I, $\mu_A 20$, η_g
6	$61.5\ 10^4$	634	$b_H 20$, fX_{BH}, fX_I, fS_I, $\mu_A 20$, η_g
7	$24.8\ 10^4$	1356	$b_H 20$, fX_{BH}, fX_I, fS_I, $\mu_A 20$, $\mu_H 20$, η_g
8	$10.5\ 10^4$	2400	$b_H 20$, fX_{BH}, fX_I, fS_I, $\mu_A 20$, $\mu_H 20$, Y_A, η_g

Some remarks should be made here. First, it is noted that the analysis reveals that the influent COD fractions fX_I and fS_I can be estimated from output measurements together with other parameters. This differs from many procedures applied, where often S_I is estimated separately from effluent COD alone, which may consequently introduce bias.

Second, with the determinant as sole criterion, very similar subsets are obtained, with the notable exception of Y_H. This parameter causes high condition numbers and at the same time high determinants. More careful

analysis revealed that for almost all outputs of the output set used, the sensitivity for Y_H was high. This causes the main diagonal element of the Fisher matrix corresponding to Y_H to be higher than for other parameters. This leads to a relatively large eigenvalue, which in turn leads to high condition numbers and large determinants. Thus the high sensitivity towards Y_H leads to accurate estimates of this parameter. From this consideration it must be concluded that it is advisable to include Y_H in the set of parameters to be estimated, as even small errors introduced by assuming this parameter to be known might lead to large errors in other parameters. However, including this parameter in the set may lead to larger numerical problems during estimation, because of worse conditioning.

Results of testing the selection procedure

1. Test by estimating from simulated data with known 'true' parameter values

The parameter subsets of Table 1 were estimated from simulated data without noise. In the estimation, a parameter scaling was applied, in order to improve numerical properties and reduce differences in relative accuracy for the parameters. The values assumed in the starting point were used for scaling. Up to the set containing seven parameters, the estimation was within the specified relative accuracy of 0.1%. Reliability was checked by using different search algorithms and initialising them with different starting points. With the 8 parameter subset, small deviations started to occur, in the order of magnitude of 1% (results not shown).

Subsequently, parameters were estimated from simulated data with noise levels of 5% of the mean output values (Gaussian white noise). The results for different parameter subset sizes are shown in Table 2, expressed as relative deviation from the known 'true' values in percents which is possible because the true values are known. Here also two different starting points were used for most set sizes. For both tables, the relative accuracy of the estimates is within 5% for sizes up to 5 parameters. For larger size of 6 up to 8 parameters, deviations of approximately 10% started to occur in the least sensitive parameters. From this result and from the result without noise, it was decided to set the maximum subset size at 8 parameters.

Table 2. Results of estimation of parameter subsets selected with combined criterion from simulated data with noise, presented as relative deviation (%) from known 'true' value

N	Starting point†	Parameters							
		fX_I	$\mu_A 20$	fS_I	b_H	η_g	fX_{BH}	$\mu_H 20$	Y_A
2	1, 2	0.30	-0.18						
3	1, 2	0.53	-0.10	2.64					
4	1, 2	0.91	-0.14	2.79	0.73				
5	1, 2	1.89	-0.24	-2.10	-0.15	1.96			
6	2	-1.33	-1.42	-1.48	3.40	0.025	-9.60		
7	1	-3.34	-1.27	1.50	4.82	-3.19	-10.11	8.70	
	2	-3.29	-1.27	1.33	4.74	-3.02	-10.09	8.20	
8	1	-4.50	0.70	1.81	4.34	-4.04	-10.36	9.63	3.29
'True' point		0.398	1.000	0.0604	0.620	0.800	0.700	4.00	0.240
† Starting point 1		0.358	0.900	0.0544	0.558	0.720	0.630	3.60	0.216
Starting point 2		0.239	0.600	0.0400	0.372	0.600	0.700	2.40	0.144

2. Test by estimating from real data

The selected parameter subsets for set sizes up to 5 parameters were estimated from real data (Table 3). The results are given as estimated parameter values, because no relative deviations can be computed as the true values are not known. From the results per subset size, it can be seen that almost the same optimal parameter set was found with different starting points and estimation methods. As unique parameter values were obtained, this confirms that these subsets were indeed identifiable, as was concluded from the selection criterion used. It is remarkable that this result is obtained despite the fact that the Fisher information matrix has only local validity and differences up to 100% of the *a priori* assumed values occur.

On the other hand, the results of Table 3 also show that the values obtained for a particular parameter are dependent on the total number of estimated parameters. This can be explained as follows. When estimating a set of parameters, the other, non-estimated parameter values have to be assumed. Errors in the assumed

parameters are compensated for by the errors in the estimated parameters. If the parameter subset increases in size, less parameter values are assumed and the distribution of the errors over the parameters changes, resulting in a change of all parameter estimates. This shows that estimated parameter values are not mutually independent even though by the selection criterion used they were selected on minimal interdependency, so one has to be careful in assigning a physical meaning to parameter values obtained. Increasing the subset size to 6 or more parameters resulted in non-realistic parameter estimates. This was not predicted by the test results with the simulated data and is most probably caused by model mismatch, which was significant in this case due to different causes. This model mismatch may lead to unrealistic parameter values, as wrong model structure is (partly) compensated for by erroneous parameter estimates. For more definite conclusions on the number of practically identifiable parameters, more detailed study is required.

Table 3. Results of estimation of parameter subsets selected with combined criterion from real data

N	Starting point†	Method‡	Parameters				
			fX_I	$\mu_A 20$	fS_I	b_H	η_g
2	1, 2	S, LM	0.450	1.195			
3	1, 2	S, LM	0.440	1.192	0.0746		
4	1	S, LM	0.274	0.878	0.0841	0.173	
	2	LM	0.274	0.878	0.0841	0.173	
5	1	S, LM	0.351	0.863	0.0871	0.155	1.158
	2	LM	0.351	0.863	0.0871	0.156	1.152
† Starting point 1			0.398	1.000	0.0604	0.620	0.600
Starting point 2			0.239	0.600	0.0400	0.372	0.600

‡ S: Simplex, LM: Levenberg-Marquardt

Another exercise reported in more detail in Weijers *et al.* (1996) consisted of evaluating subsets selected with the determinant as ranking criterion. With this ranking only up to 4 parameters could be estimated from the output set chosen. This was to be expected, because the condition numbers are worse and hence the identifiability properties are less good. It is too early, however, to conclude that the combined criterion is to be preferred as it is advisable to estimate Y_H for the reasons indicated above.

3. Test sensitivity to a priori assumption by applying Latin hypercube sampling

The selection of reduced parameter sets and of best identifiable parameter subset, step 2 and 3 in the procedure given above, were repeated with the 23 parameters considered relevant. From the literature and experience, ranges considered realistic were defined for all of these parameters. The ranges defined are given between square brackets: Y_h[0.55-0.67], f_p[0.08-0.2], Y_a[0.1-0.25], μ_{h20}[2-10], K_s[2.5-20], K_{oh}[0.1-1], K_{nhh}[0.02-0.2], b_{h20}[0.1-1.5], η_g[0.6-1.0], η_h[0.35-0.4], K_{no}[0.1-0.5], k_{h20}[2-4], K_{x20}[0.03-0.15], k_{a20}[0.016-0.8], μ_{a20}[0.2-1.2], K_{nha20}[0.8-10], K_{oa}[0.1-1]; b_{a20}[0.04-0.15], fS_i[0.04-0.2], fS_s[0.05-0.25], fX_s[0.4-0.6], fX_i[0.05-0.4], fX_{bh}[0.01-0.2], f_{Xba}[0.001-0.01].

115 parameter points were sampled, each of these representing a particular point in 23-dimensional parameter space and thanks to the LHS sampling design guaranteed to cover the whole space. For all 115 parameter points, sensitivity functions of the five outputs with respect to all 23 parameters were computed. Then reduced sets were determined by applying method (i) described in the procedure section (compute time-averaged output sensitivities, scale by the maximum output sensitivity, select reduced sets consisting of all parameters with at least one scaled output sensitivity value larger than 0.2). The occurrences within the reduced sets thus obtained for the 115 different LHS parameter sets were as follows (ranked according to the number of occurrences): fS_i 115, μ_{a20} 115, Y_a 115, Y_h 115, η_g 111, K_{nha20} 95, K_{oa} 88, b_{h20} 85, k_{h20} 79, K_{oh} 62, fX_i 39, μ_{h20} 29, K_{x20} 18, K_{no} 16, K_s 16, η_h 10, fS_s 5, k_{a20} 1, fX_{ba} 0, fX_{bh} 0, b_{a20} 0, K_{nhh} 0, f_p 0. Although these results indicate an order of importance, it was observed that with the selection criterion used (value > 0.2), the size of the reduced set varied too severely, namely from 4 to 15 parameters depending on the LHS parameter set considered. It thus appears that this criterion is not effective for reducing the set to a consistent set of important parameters that would hold independent of the *a priori* assumption of the parameter values. To accommodate for this, method (ii) for step 2 of the procedure was chosen, which also agrees better with the behaviour of the least squares criterion used within estimation as it does not artificially change the sensitivity of an output by scaling with the maximal sensitivity of that output. This alternative consists of

omitting the scaling by the maximal sensitivity for each output and instead, ranking the parameters according to the sensitivity coefficients, averaged over the 5 outputs. In Figure 2, the rankings thus obtained within the individual LHS samples are plotted as a function of the sampling number for the 6 most sensitive parameters.

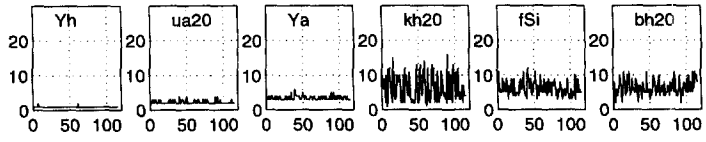

Figure 2. Parameter ranking over the LHS sample if ranked according to mean sensitivity over the outputs.

These plots have been organised from left to right ordered by a second ranking, which consists of averaging the output-averaged sensitivity coefficients over the 115 LHS samples and ranking the parameters and corresponding plots in descending order of this LHS-sample-averaged sensitivity.

In Figure 3 the results are summarised as histograms of the rankings for all of the parameters. Also these histograms have been organised from top left to bottom right in descending order of LHS-sample-averaged sensitivity. It can be observed that if about 14 parameters are selected, the most important are consistently present. This means that the set can indeed be reduced, and a size of 14 appears adequate. What can also be observed is that some parameters show a much larger variation in their relative sensitivity than other parameters. This especially holds true for k_h, K_{nha}, fX_i and to a lesser extent for K_{x20} and μ_{h20}. Hence, with respect to the latter parameters the composition of the reduced set seems to depend on the *a priori* assumed values. Some of the other parameters such as f_p, $_h$, fX_{bh} and fX_{ba} show a large variation in sensitivity, but are always in the range of least sensitive parameters and consequently can be omitted consistently.

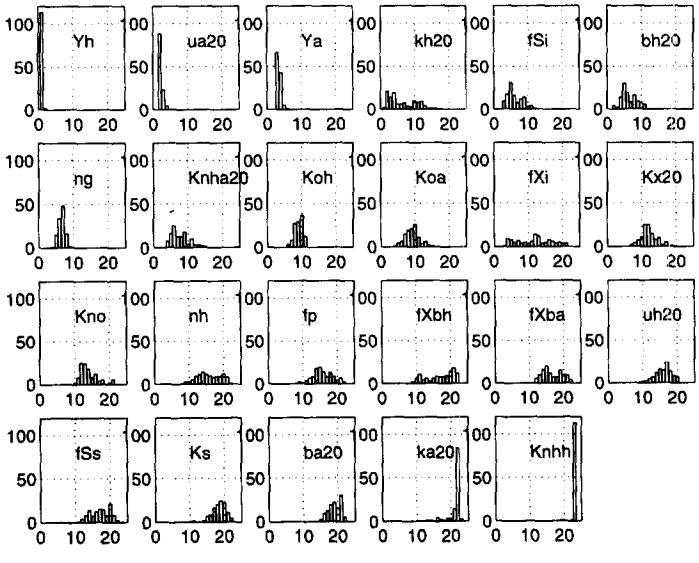

Figure 3. Histograms of occurrences of ranking positions of parameters.

Finally, parameter subset compositions were determined over the LHS sample, after first reducing the set to 14 parameters. A subset size of 8 parameters was chosen, and the determinant of the Fisher information matrix was used as the selection criterion. This choice was made, because the heuristic procedure used with the combined criterion considering both the condition number and the determinant does not lend itself to

straightforward ranking, which was required to analyse the large sample used. The occurrences of parameters in the subsets obtained was as follows: Y_h 115, k_{h20} 115, fS_i 115, μ_{a20} 114, b_{h20} 100, K_{no} 88, η_g 82, fX_i 61, Y_a 38, K_{oh} 37, K_{x20} 32, K_{nha20} 23, K_{oa} 0, η_h 0. This shows that the same 5 parameters Y_h, k_{h20}, fS_i, μ_{a20} and b_{h20} in the subsets obtained in almost all of the samples, and K_{no}, η_g and fXi in most of the subsets, indicating that the subset size composition is not substantially changed by the *a priori* assumption on the parameter values.

The results obtained with LHS sampling indicate that the procedure can be applied to obtain identifiable parameter subsets. The number of identifiable parameters was limited (to 8), however, which means that not all important parameters can be estimated with the output set defined. Errors in non-estimated, fixed parameters may then lead to errors in estimated parameters, especially because non-selected parameters can have a strong interaction with selected parameters; in fact, this is the reason they are rejected in the identifiable subset selection step. To get around this problem, more outputs and/or dedicated experiments yielding information on these parameters have to be looked for. The selection procedure proposed can be utilised for this task as well.

CONCLUSIONS

A procedure was suggested for selecting important and identifiable parameter subsets for calibrating ASM1. This procedure utilises sensitivity functions and the Fisher information matrix. However, these are local properties in parameter space and consequently may depend upon an *a priori* assumption on parameter values which has to be made. Therefore, the procedure was tested by estimation on simulated as well as measured data, which indicated that the procedure was successful in selecting identifiable subsets. In addition, a Latin hypercube sampling procedure covering the whole parameter space showed that the results obtained by the procedure are not too strongly influenced by the *a priori* assumption. This means that a tool has been developed which is helpful in selecting parameters that can be uniquely estimated from the data available. The next challenge is now to use this approach to find optimal experimental designs which optimally combine full-scale plant input/output data with dedicated experiments, especially respirometry, in order to obtain all relevant parameters.

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