Discussion of "Assessing Parameter Identifiability of Activated Sludge Model Number 1" by Pedro Afonso and Maria da Conceição Cunha

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Parameter identification, as discussed by the authors, is a very important task within modeling, and particularly, model calibration. We would like to congratulate the authors for their contribution to this field. However, in order to increase the understanding of this rather complicated modeling task we would also like to bring forward some points of discussion.

As a first point we would like to stress that a clear distinction should be made between structural and practical identifiability.

The structural identifiability as a first step addresses whether there is any chance of obtaining a unique value for the parameters, given the structure of the model and the measurements to be performed. Structural identifiability can be performed in the absence of any prior information on the value of the parameters and even before collecting any data on the system to be studied. Many techniques exist to assess the structural identifiability (Walter and Pronzato 1997), including the technique used by the authors, the "numerical local approach," in which noise-free data is used to assess the identifiability of the parameters by trying to estimate potential identifiable parameters to a generated set of noiseless data. However, it should be noted that this technique can only be used to assess the local structural identifiability of a parameter and not its global identifiability, as presented by the authors.

The practical identifiability of parameters, on the other hand, depends not only on the model structure, but also on the experimental conditions together with the quality and quantity of the measurements. It gives an assessment of the accuracy with which parameters can be estimated. Most methods for the evaluation of practical identifiability are based on the parameter estimation covariance matrix or its inverse, the Fisher Information Matrix (see Dochain and Vanrolleghem 2001). Note that, if parameters are practically identifiable, they are also locally structurally identifiable, and that is the essence of the numerical local approach. However, it means that the accuracy of these parameter estimates must be evaluated too, something not done by the authors.

The authors investigated the structural identifiability of ASM1 using the numerical local approach. A number of parameter estimation algorithms were used, including gradient- and nongradient-based methods. From the results the authors reported that the algorithms did not converge for some situations. To us, it is not very clear what the authors meant by nonconvergence. Was it because the parameters were correlated and the parameter estimation algorithm stopped at a local minimum or was it caused by numerical problems of the algorithms. It would also be very interesting to know if different sets of initial parameter values were used and what the values of the final estimates and their variances were. This is a very important and well-known check of the identifiability of parameters as expressed by the uniqueness of the parameters.

In the introduction of the identification algorithms, the authors mentioned that numerical problems were to be expected with the gradient-based method. Dochain and Vanrolleghem (2001) also list a number of authors who have found poor convergence for the Levenberg-Marquardt algorithm. In contrast to that statement, it was found that the Levenberg-Marquardt (gradient-based) method performed best. Important to mention is that Walter and Pronzato (1997) suggested not to use the Levenberg-Marquardt for local structural identifiability analysis because of the regularization procedure used in the algorithm.

The authors conclude that a large number of parameters (up to 15) are structurally identifiable from oxygen measurements alone, including the yield coefficient. However, from the (many) structural identifiability analyses that have been performed with ASM-type models using only oxygen measurements (e.g., Dochain et al. 1995; Petersen et al. 2001), it was concluded that only combinations of parameters with the yield coefficient (Y_H), maximum growth rate (μ_{max}), substrate half-saturation coefficient (K_{SH}), and initial biomass concentration (X_H) could be structurally identified. The claim made in the paper that up to 15 parameters can be identified uniquely using only oxygen measurements is therefore very questionable. The fact that 15 parameters get a value in a numerical parameter estimation procedure does not imply structural identifiability. Parameters of a model that is not structurally identifiable can indeed get values, but these are not unique, and that is the property to evaluate. Rather than going into a theoretical discussion, the point is illustrated in Fig. 1 and Fig. 2 for the aerobic oxidation of COD. The simplified COD mass balance only considering the aerobic heterotrophic COD oxidation process [neglecting the dynamics (kinetics) of the process] is given by Eq. (1):

$$\Delta S_S = \Delta X_H + \Delta S_{O,H} \tag{1}$$

where $\Delta S_S = (S_{S,\text{in}} - S_S)$. And

$$\Delta X_H = Y_H * \Delta S_S \tag{2}$$

$$\Delta S_{O,H} = (1 - Y_H) * \Delta S_S \tag{3}$$

where ΔX_H = biomass production (mg COD); $\Delta S_{O,H}$ = oxygen consumption due to heterotrophic growth (mg COD); and ΔS_S = readily biodegradable substrate oxidized (mg COD).

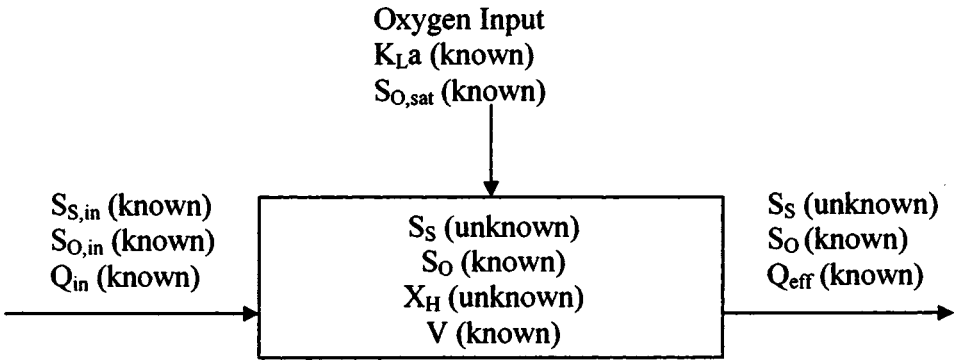

Fig. 1. COD mass balance around the aeration tank considering only the aerobic oxidation of COD by heterotrophic biomass. The oxygen transfer coefficient ($K_L a$), saturation oxygen concentration ($S_{O,sat}$) and influent characteristics (Q_{in}, $S_{S,in}$ and $S_{O,in}$ etc... .) are assumed to be known a priori, while only S_O is measured.

It can clearly be seen from Eq. (1) that the COD mass balance has two unknowns—substrate removed and biomass produced—whereas only the oxygen consumption is known. This means that Eq. (2) and Eq. (3) can be solved by any combination of $(1-Y_H)*\Delta S_S$ (Dochain et al. 1995) (see Table 1 for some examples). This simple example demonstrates why only values for combinations of parameters rather than values for the single parameters can be estimated based on oxygen measurements alone [see Dochain et al. (1995) for further explanation]. Moreover, for the full ASM1 model as studied by the authors we also need to consider the autotrophic organisms, in addition to the heterotrophic bacteria. Both organism types contribute to the oxygen consumption:

$$\Delta S_{O,\text{total}} = \Delta S_{O,H} + \Delta S_{O,A} = (1-Y_H)*\Delta S_S + (4.57-Y_A)*\Delta S_{\text{NH}} \quad (4)$$

Given only oxygen measurements, it is clear from Eq. (4) that neither Y_H nor Y_A can uniquely be identified. This brings us to the conclusion that it is impossible to uniquely identify 15 parameters given only oxygen measurements, as claimed by the authors. Thus, it can be concluded that the identifiability of each parameter of the ASM1 model depends largely on the considered measured variables (Petersen et al. 2001). It is clear that more information (e.g., NO_3 data, effluent COD, biomass production ...) about the system is required to uniquely identify the large number of parameters considered in ASM1.

As stated before, the practical identifiability is closely related to the quality and quantity of the data. This aspect is not sufficiently stressed by the authors. Calibration and identifiability studies can only be carried out if sufficient and information-rich data is available.

In order to catch all the dynamics of the treatment plant, it is advisable to take as duration of the measurements several HRTs (hydraulic retention times) as opposed to the 0.2 days of measurements used by the authors (Petersen et al. 2002). It is also preferred to have time-varying conditions in the WWTP, in contrast to the presented case where all variables stay more or less constant. We also question the choice of the sampling interval (being 7.5 min), because the suggested O_2 (DO, dissolved oxygen) measurements can be obtained using a much smaller interval (on the order of seconds). Besides O_2 and NO_3 measurements, the authors also propose to measure the readily biodegradable substrate S_S in the aeration tanks. To our knowledge, no measurement technique exists in order to measure this quantity on a full-scale plant in the mixed liquor. Therefore it should preferably not be used in a model calibration case study.

The authors present a procedure for evaluation of the practical identifiability of the ASM1 model parameters. This procedure is based on nonlinear regression analysis, which uses a sum-of-squared-errors objective function to minimize the difference between model output and measurements. Further, the Fisher information matrix, which contains the second derivatives of the objective function, is used to assess the precision of the parameter estimates. The variance of the observations is incorporated in the calculation of the Fisher information matrix by using the objective function value, the number of measurement points, and the number of estimated parameters. This approach holds only if all measurements have identical measurement error and no correlation between them exists. In our opinion this assumption does not hold (as the authors themselves accept by using a relative measurement noise) and a weighted sum-of-squared-errors objective function that incorporates the measurement error for every measured variable should be used instead. Also, the measurement error covariance matrix should be used in the calculations of the Fisher information matrix (Dochain and Vanrolleghem 2001).

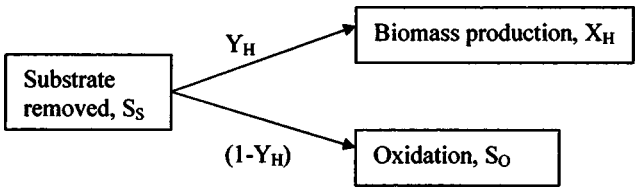

Fig. 2. Concept of yield coefficient based on COD unit

Table 1. Infinite Number of Solutions to COD Mass Balance with Only ΔS_O Known. Examples Given for $S_O = 10$ mgCOD/l and $S_{S,in} = 35$ mgCOD/l

ΔS_O mgCOD/l	$(1-Y_H)$	ΔS_S mgCOD/l	Y_H mgCOD/mgCOD	ΔX_H mgCOD/l	S_S mgCOD/l
10	0.33	30.30	0.67	20.3	4.7
10	0.50	20.00	0.50	10.0	15.0
10	0.40	25.00	0.60	15.0	10.0
—	—	—	—	—	—

In order to assess practical identifiability, the authors added noise to the data and ran the identification procedure. However, in order to avoid meaningless estimation results, boundaries were established on the parameters. From the results of the identification study it can be seen that some parameter estimates are at their bound, meaning that the ''true'' value is probably outside the parameter bounds. This typically points to model inadequacy and this should have been discussed.

In order to rule out badly identifiable parameters, a sequential selection procedure was used in which the least accurate parameter was eliminated from the set. In our opinion it would be better, as in Weijers and Vanrolleghem (1997), to investigate all possible parameter subsets because removing one parameter could influence the identifiability of the remaining parameters.

Finally, the iterative identifiability process was stopped when the estimates for the reduced set of parameters were ''close'' to the real values. It must be clear that, in practically any actual calibration study, this can never be used as a stopping criterion, for the real values of the parameters are never known. Other authors have presented different stopping criteria in similar studies (Brun et al. 2002; Weijers and Vanrolleghem 1997), and these should have been discussed.

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