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REFORMULATION METHODS FOR A HYBRID PARAMETER ESTIMATION PROBLEM

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ABSTRACT

We study the dynamic parameter estimation problem for a hybrid system where the continuous evolution interacts with discrete switching processes. The latter can be due to external control actions as well as internal mode transitions. Dynamic parameter estimation can be considered as a constrained nonlinear optimization problem. The solution of such a problem faces the difficulty that for hybrid systems the objective function and the state trajectories can be nonsmooth or even discontinuous. Particularly promising are reformulation strategies that aim at removing nonsmoothness from the optimization problem. We investigate two conceptually quite different reformulation methods for a three-tank system. Penalization of incomplete switching (PICS) introduces a penalty term into the objective function. Smoothing of the step function (SSF) replaces the instantaneous transition by a rapid, but continuous one. Here, a new functional form is suggested for the switching function. For both methods, the accuracy, the robustness against error in measurement, and the dependence of the solution on the details of the respective reformulation are investigated.

Index Terms— parameter estimation, optimization of hybrid systems, reformulation methods

1. INTRODUCTION

Parameter estimation is an important issue in many fields of industrial research [1], since it allows for efficient adaptation of system models. Accurate models are a prerequisite for optimization in almost every sector of technology. Dynamic processes can be described by differential algebraic equations. However, in many technical systems there exist autonomous mode transitions or control actions [2, 3]. As a consequence, the behavior of the system cannot be considered as completely continuous but contains switching of the structure or the driving mode: The time evolution of the states is given by periods of continuous evolution in a certain mode seperated by instantaneous transitions between different modes. Such systems with mixed continuous and discrete behavior are called hybrid systems.

Parameter estimation aims at extracting the best values of the parameters determining the dynamics of the system under consideration based on a series of measurements $x_{ij}^{(m)}$ of several state variables x_i, $i = 1...M$ at different points in time t_j, $j = 1...N$. In engineering, parameter estimation is almost exclusively implemented as optimization problem minimizing the objective function $\mathcal{J}$ given by the squared deviation

$$\mathcal{J}(p) = \sum_i^M \sum_j^N (x_i(t_j) - x_{ij}^{(m)})^2 \,. \qquad (1)$$

Here, $x_i(t_j)$ are the model values derived, e. g. by solving the differential equations with a given set p of parameter values. Thus, $\mathcal{J}$ depends implicitely on p. Minimizing $\mathcal{J}$ with respect to p provides in the least-square sense the best estimation of the parameters. The present work adresses the issue of how to treat numerically the multidimensional parameter estimation problem or, more generally, the optimization problem with underlying hybrid dynamics. Taking into account the hybrid nature of real industrial systems, various challenges remain for multidimensional dynamic parameter estimation. First, there can be problems connected to the least-square method itself [4, 5]. Beside mathematical programming, different heuristic approaches were investigated [6, 7]. Second, since we deal with dynamic models, the necessary discretization converts the contraints to a large-scale nonlinear system of equations [8, 9]. Third and this is the main focus of this contribution, the hybrid nature may lead to discontinuities in the objective function, the contraints and/or their gradients. In order to make the hybrid problem accessible for well established NLP solvers, reformulations of the hybrid model are necessary. However, the reformulation must retain the hybrid feature in some way. This in general leads to a tradeoff of accuracy vs. stability and robustness of the optimization algorithm. The reformulation methods presented here introduce a continuous switching variable to provide the correct switching behavior. This variable is forced to meaningful values through penalization of incomplete switching (PICS)

[10, 11] or smoothing of the step function (SSF). The idea of a smoothing function goes back to Ref. [12]. To the best of our knowledge, the specific form of the smooth step function is suggested first in this contribution. The article is organized as follows. In section 2, we will introduce the reformulation methods for hybrid optimization problems. Section 3 presents the model of a three-tank system which is chosen to demonstrate the capability of the reformulation methods to solve a parameter estimation problem with hybrid dynamics in a specific case. Sections 4 and 5 show optimization results using the method of PICS and SSF, respectively. Section 6 compares both methods regarding the magnitude of the objective function, the accuracy of the obtained parameter values, and the ability to find correct switching times. Section 7 summarizes the paper.

2. OPTIMIZATION OF HYBRID SYSTEMS

Much effort went into the simulation of hybrid dynamic models [13] due to their huge importance for technical systems. These systems can be treated succesfully by determining switching points and restarting (continuous) simulation with new initial conditions at these points [14]. In contrast, in dynamic optimization this approach is not practicable, since we need to discretize the system, but do not know the switching points and active modes, i.e. the differential equations to be solved at that time epoche in advance. As mentioned above, instantaneous changes of the dynamics cause discontinuities in the objective function, the constraints or their gradients. As a consequence, Lagrange multipliers are not necessarily bounded and the constraints are not linearly independent. Thus, the linear independence contraint qualification (LICQ) and the Mangasarian-Fromovitz constraint qualification (MFCQ) will be violated in these nonsmooth systems [10]. In spite of these problems, some progress was made, e.g., in Model Predictive Control (MPC) of these kinds of systems [3, 15]. Various methods of regularization and Mixed Integer Programming were used [10, 16, 17]. Particular promising are reformulation strategies that aim at removing nonsmoothness from the optimization problem [11]. This may imply that the solution of the reformulated problem yields only an approximate description of the original system. In this contribution, we investigate two conceptually quite different reformulation methods. In case of a binary hybrid system, the optimization problem can be desribed by

$$\begin{aligned} \min \quad & \mathcal{J}(x,u,p) && (2)\\ \text{s.t.} \quad & \\ \dot{x} \; &= f^{(1)}(x,u,p), \quad s(x,u,p) \geq 0 \\ \dot{x} \; &= f^{(2)}(x,u,p), \quad s(x,u,p) < 0 \\ & x_l \leq x \leq x_u,\; u_l \leq u \leq u_u,\; p_l \leq p \leq p_u \end{aligned}$$

where $\mathcal{J}(x,u,p)$ is the objective function which may depend on the state variables $x(t)$, the control variables $u(t)$ and the parameters p. The equality contraints $\dot{x} = f^{(\mu)}(x,u,p)$, $\mu = 1,2$ reflect the dynamics of the system, which evolves in mode 1, if some switching function $s(x,u,p) \geq 0$ and in mode 2, otherwise. In addition, all variables might be bounded. The key step in our reformulation approach is the introduction of a continuous switching variable $\sigma(t) \in [0,1]$ which connects both modes in a single set of equality constraints. Now, the optimization problem reads

$$\begin{aligned} \min \quad & \mathcal{J}(x,u,p) && (3)\\ \text{s.t.} \quad & \\ \dot{x} \; &= \sigma \cdot f^{(1)}(x,u,p) + (1-\sigma) \cdot f^{(2)}(x,u,p) \\ 0 \; &\leq \sigma \leq 1 \\ & x_l \leq x \leq x_u,\; u_l \leq u \leq u_u,\; p_l \leq p \leq p_u \end{aligned}$$

For real switching between the two modes, the variable σ can only have the value 0 or 1, since only one mode can be active at any given time. To achieve this behavior we accomplish the reformulation according to PICS or SSF, respectively. In PICS, an inner optimization problem

$$\begin{aligned} \min_{\sigma} \quad & -s \cdot \sigma && (4)\\ \text{s.t.} \quad & \\ \dot{x} \quad &= \quad \sigma \cdot f^{(1)}(x,u,p) + (1-\sigma) \cdot f^{(2)}(x,u,p) \end{aligned}$$

is introduced. The inner objective function $-s \cdot \sigma$ is minimized for $\sigma(t) = 1$ if $s \geq 0$, whereas $\sigma(t) = 0$ minimizes this product in case of $s < 0$. For the optimization problem (4) we write the Karush-Kuhn-Tucker (KKT) conditions in terms of non-negative Lagrange multipliers λ_0, λ_1 as

$$\begin{aligned} 0 &= -s - \lambda_0 + \lambda_1 && (5)\\ 0 &= \lambda_0 \sigma \\ 0 &= \lambda_1 (1-\sigma) \\ 0 &\leq \lambda_0,\, \lambda_1 \,. \end{aligned}$$

The complementary constraints in equation (5) can either be relaxed [10] or incorporated into the upper objective function as a penalty term as it is done here. The penalized objective function

$$\min \; \mathcal{J}(x,u,p) + \rho \int_{t_0}^{t_f} (\lambda_0 \sigma + \lambda_1 (1-\sigma))\, dt \quad (6)$$

contains the weighting parameter ρ, which must be chosen with care. For very small ρ, the weak penalization allows constraint violation to some extent. Hence the switching variable σ is not sufficiently driven towards 0 or 1. If ρ is too large, the penalization overwhelmes the original objective function making it exceedingly difficult in actual application to find the almost discontinuous trajectory $\sigma(t)$.

In the SSF method we give up the strict complementarity of modes but approximate it by means of the smoothened step function

$$\sigma = \frac{1}{1 + \exp(-\tau s)} \tag{7}$$

which reproduces the instantanuous switch in the limit of large step slope τ.

3. PARAMETER ESTIMATION IN A MODEL HYBRID SYSTEM

To examine the performance of the reformulation methods, we consider a three-tank system (Fig.1), since it is simple enough to understand its behavior intuitively but exhibits non-trivial hybrid properties. There are inflows Q_{zi}, $i = 1, 3$ to the left and the right tank. The

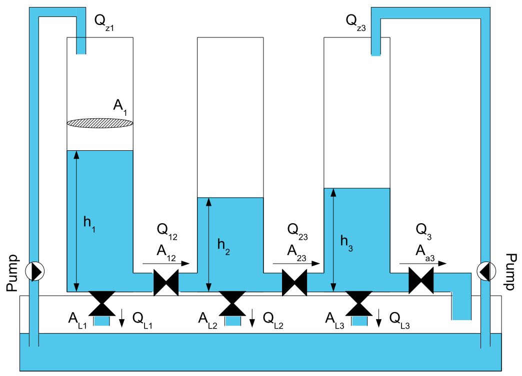

Fig. 1. *Three-tank system. If not noted otherwise, we used parameters* $A_i = 0.0149\, m^2$ $(i = 1, 2, 3)$, $A_{L1} = 6.0 \cdot 10^{-5}\, m^2$, $A_{L2} = 0$, $A_{L3} = 0.1 \cdot 10^{-5}\, m^2$, $A_{a3} = 1.0 \cdot 10^{-5}\, m^2$, $Q_{z1} = 10 \cdot 10^{-5}\, m^3$, $Q_{z3} = 5 \cdot 10^{-5}\, m^3$. *The flow parameters* A_{12} *and* A_{23} *which represent the area of the connecting tube between the tanks in each case are estimated based on the measurement of one tank level.*

dynamics of the tank levels h_i, $i = 1, 2, 3$ is given by

$$
\begin{aligned}
A_1 \dot{h}_1 &= Q_{z1} - Q_{12} - Q_{L1} && (8)\\
A_2 \dot{h}_2 &= Q_{12} - Q_{23} - Q_{L2} \\
A_3 \dot{h}_3 &= Q_{z3} + Q_{23} - Q_{L3} - Q_3 \\
Q_{ij} &= A_{ij} \operatorname{sign}(s_{ij}) \sqrt{2g|s_{ij}|} && (9)\\
s_{ij} &= h_i - h_j, \quad (i,j) = \{(1,2),(2,3)\}\,.
\end{aligned}
$$

The flows between the tanks Q_{ij} and analogously the outflows Q_{Li}, Q_3 are modeled by Toricelli's law. The sign function $\operatorname{sign}(h_i - h_j)$ switches the direction of the flow between two tanks abruptly from $+1$ to -1 or vice versa, when the condition $s_{ij} = h_i - h_j = 0$ is passed. Therefore, the gradient of the flow diverges to infinity at this point.

As a paradigmatic example of parameter estimation for hybrid systems, we estimate the parameters A_{ij} based on assumed measurement data of the tank levels. The data are generated via simulation of the original model (eq. 8) with $A_{12} = 6.0 \cdot 10^{-5}\, m^2$, $A_{23} = 2.0 \cdot 10^{-5}\, m^2$ and added gaussian noise. We use the data of level h_1 in PICS and h_3 in SSF. Thus, the objective function reads

$$\mathcal{J} = \sum_j^N (h(t_j) - h_j^{(m)})^2\,. \tag{10}$$

The equality constraints representing the system dynamics are reformulated according to sec. 2

$$Q_{ij} = A_{ij} \hat{\sigma}_{ij} \sqrt{2g|s_{ij}|}, \; (i,j) = \{(1,2),(2,3)\} \tag{11}$$
$$-1 \leq \hat{\sigma}_{ij} \leq 1$$

with the switching variable $\hat{\sigma}_{ij} = 2\sigma - 1$, $\hat{\sigma}_{ij} \in [-1, 1]$. The PICS equality constraints are the KKT conditions of the inner minimization problem

$$
\begin{aligned}
0 &= h_j - h_i - \lambda_{10} + \lambda_{11} - \lambda_{20} + \lambda_{21} && (12)\\
0 &= \lambda_{10}(1 + \hat{\sigma}_{12}),\; 0 = \lambda_{11}(1 - \hat{\sigma}_{12}) && (13)\\
0 &= \lambda_{20}(1 + \hat{\sigma}_{23}),\; 0 = \lambda_{21}(1 - \hat{\sigma}_{23}) && (14)\\
0 &\leq \lambda_{10}, \lambda_{11}, \lambda_{20}, \lambda_{21}\,. && (15)
\end{aligned}
$$

The complementarity of the Lagrange multipliers eq. (13, 14) is then incorporated into the objective function as a penalty. The equality constraints of the the SSF approach are given by eq. (8) with expression (11) and the smoothened step function (7).

4. PENALIZATION OF INCOMPLETE SWITCHING

In this section we present the results of the parameter estimation with PICS. Figure 2 shows the simulation result for the state variables h_i, the measurement data of h_1 and the trajectories of h_i at the PICS solution. We use one data series with noise variance $\sigma_M = 0.005\, m$ and the penalization parameter $\rho = 7.8 \cdot 10^{-6}\, m^2 s^{-1}$. As seen in Fig. 2, the measurements are well fitted by the trajectory of h_1. The parameter values were found to be $A_{12} = 5.9 \cdot 10^{-5}\, m^2$ and $A_{23} = 2.5 \cdot 10^{-5}\, m^2$. The true values are $A_{12}^{(true)} = 6 \cdot 10^{-5}\, m^2$ and $A_{23}^{(true)} = 2 \cdot 10^{-5}\, m^2$. Apparently, the parameter A_{12} can be estimated more precisely. Switches of the flow direction occur at the crossing points $h_1 - h_2 = 0$ and $h_2 - h_3 = 0$. The corresponding switching variables displayed in Fig. 2b reflect this correctly. The flow direction $\operatorname{sign}(Q_{12})$ is controlled by means of σ_{12} which is 1 at the beginning and changes its value to -1 at about $t = 15.5\, s$. For the flow Q_{23}, the switching variable σ_{23} starts at -1, since $h_3 > h_2$, changes to +1 at $t = 2.5\, s$ and returns to -1 at $t = 18\, s$.

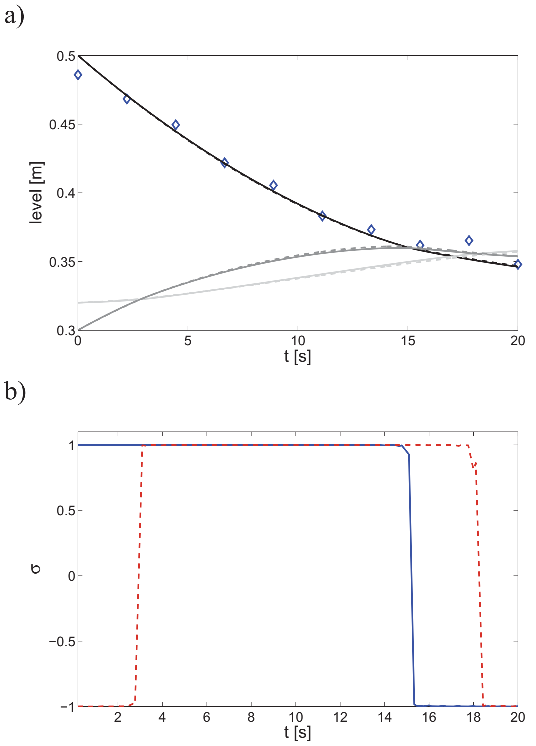

Fig. 2. *PICS solution of the parameter estimation with $\rho = 7.8 \cdot 10^{-6}\, m^2 s^{-1}$ and $\sigma_M = 0.005\, m$. a) State trajectories h_1 (black), h_2 (dark grey) and h_3 (grey) at the solution (solid) compared to the underlying simulation (dashed) and derived measurement data for h_1 (diamond). b) Trajectories of the switching variables $\hat{\sigma}_{12}$ (solid) and $\hat{\sigma}_{13}$ (dashed). The switches are produced correctly at the crossing points of the trajectories seen in panel (a).*

It turns out that even though we are able to find good approximate parameter values, care must be taken regarding the choice of the penalty parameter ρ. The values of the objective function for several values of ρ and vanishing error in measurement σ_M are plotted in Fig. 3. For $\rho < 5.5 \cdot 10^{-6}\, m^2 s^{-1}$ (not shown), the value of the objective function is quite high ($\mathcal{J} \sim 10^{-2}\, m^2$), i.e. h_1 does not fit the measured data. Even though small values of the objective function are obtainded for the full range of ρ values shown in Fig. 3, widely varying values are found for the parameters. This could be traced back to the fact that the trajectories of the switching variables σ tend to oscillate. This is presumably due to the collocation method, which we used for the discretization of the differential equation. Taking good switching behavior, i.e. non-oscillating $\sigma(t)$ as additional criterion, values of ρ in the range $\rho = [7.5, 8.5] \cdot 10^{-6}\, m^2 s^{-1}$ seem to be the best in our example.

Some tests with $\sigma_M \neq 0$ indicate the robustness of the algorithm in presence of random error.

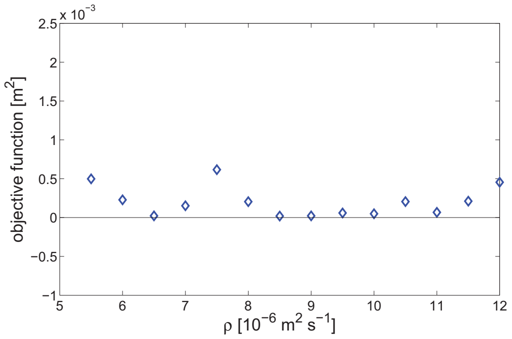

Fig. 3. *Dependence of the value of the PICS objective function on the reformulation parameter ρ.*

5. SMOOTHENING OF THE STEP FUNCTION

For the study of SSF regarding our parameter estimation problem, measurement data for the level h_3 are generated as before (see sec. 4). In Fig. 4a the simulated trajectories of all state variables h_i, $i = 1, 2, 3$, measurement data for h_3 as well as the trajectories at the SSF solution are shown. The trajectory of h_3 at the solution coincides very well with the underlying simulation. Again, we have three switching points. Here, the switches occur around $t_1 = 2.5\, s$, $t_2 = 12\, s$ and $t_3 = 14.5\, s$, respectively. They nearly coincide with those of the underlying simulation ($2.5\, s, 12.5\, s, 14.5\, s$). The switching variable by SSF is plotted in Fig. 4b. Obviously, no switch takes place instantaneously with this type of reformulation. The transition from 1 to 0 for σ_{12} needs more than $5\, s$. For the flow Q_{23}, no complete switching is obtained for, e.g. $\tau = 100\, m^{-1}$ during the whole time span, since we find only very small differences $s_{23} = \Delta h_{23} = h_2 - h_3 \approx 10^{-2}\, m$. Somewhat surprisingly, the parameter values, in particular A_{12} found in the parameter estimation by means of SSF ($A_{12} = 6.01 \cdot 10^{-5}\, m^2$, $A_{23} = 4.23 \cdot 10^{-5}\, m^2$) are quite close to the true values. We can explain this as follows. In the case of our specific model, the time points of $\sigma_{ij}(\Delta h = 0) = 0.5$ generate a correct switch, since the contributions of both modes cancel exactly. The coexistence of both modes (forward and backward flow) for $\sigma_{ij} \neq 0.5$ results in a reduced net-flow in the direction of the predominant flow, i.e. forward flow, if $\sigma_{ij} > 0.5$ and backward flow if $\sigma_{ij} < 0.5$. The reduction of the flow calls for higher values of the flow parameters. In fact, both flow parameters are overestimated.

A crucial step in this SSF implementation is the choice of the parameter τ. Figure 5 shows that the objective function value decreases strongly with increasing τ, falling below $10^{-7}\, m^2$ for $\tau > 50\, m^{-1}$. The good agreement of SSF trajectories and the underlying simulation is seen, e.g., for $\tau = 100\, m^{-1}$ in Fig. 4a. Further increase of τ does not result in appreciable a)

b)

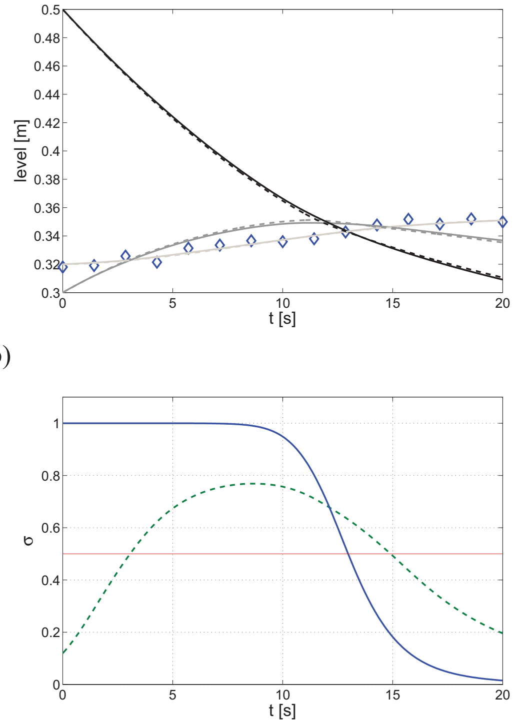

Fig. 4. *SSF solution of the parameter estimation with $\tau = 100\,m^{-1}$, $\sigma_M = 0.002\,m$ and $Q_{z1} = 5 \cdot 10^{-5}\,m^3$. a) State trajectories h_1 (black), h_2 (dark grey) and h_3 (grey) at the solution (solid) compared to the underlying simulation (dashed) and derived measurement data for h_3 (diamond). b) Trajectories of the switching variables σ_{12} (solid) and σ_{13} (dashed). The switching variables $\sigma_{12}\,\sigma_{13} = 0.5\,m$ at the crossing points of the state trajectories in panel (a) lead to zero net-flow correctly.*

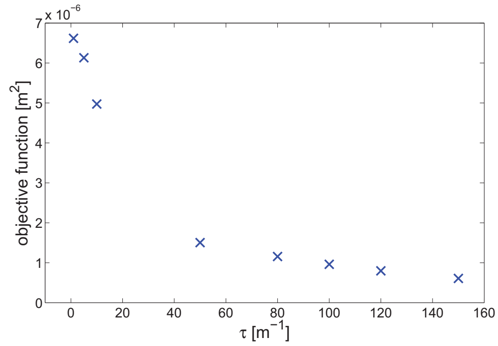

Fig. 5. *Dependence of the SSF objective function on the smoothing parameter τ with $\sigma_M = 0$.*

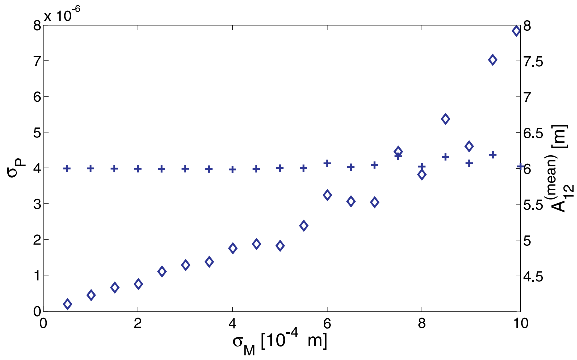

Fig. 6. *Mean parameter value $\bar{A}_{12}$ (crosses) and corresponding standard deviation σ_p (diamonds) in dependence on the variance of measurement σ_M.*

improvement of either trajectories or estimated parameters (not shown).

In order to check the ability of the SSF algorithm to cope with random error in the data set, which is inevitable in real data aquisition, the variance of the measurement is varied in the range $\sigma_M = [0.5, 10]{\cdot}10^{-4}\,m$. Parameter estimation was carried out for 50 series of h_3 for each σ_M and the mean parameter values as well as their standard deviation σ_p are calculated (see Fig. 6). The mean values of the parameter stay constant over a wide range of random error. Obviously, the higher variance of measured data leads to the higher standard deviation of the estimated parameter value. A strict proportionality of σ_M and σ_p is expected in the case of the measured quantity (here h_3) depending linearly on the parameter (here A_{12}).

6. COMPARISON OF PICS AND SSF

Comparing the results of PICS with that of SSF we find that with SSF the objective function at the optimum is up to two orders of magnitude lower than with PICS and the corresponding value of the parameter A_{12} is closer to the true value. This result is rather surprising, since the switching of the flow direction is modeled appropriately by PICS, whereas in SSF both modes are active at the same time which reduces the net-flow around the switching points as discussed in sec. 5. On the other hand, the parameter A_{23} is estimated much better by PICS. In both methods we found a higher deviation from the true value for A_{23}. Simulation reveals that the objective function is much more sensitive to A_{12} than to A_{23}. The results in secs. 4 and 5 show switching behavior and the algorithm is able to find the correct switching points. The value of the objective function at the solution depends in both methods on the respective reformulation parameter, i.e. the weighting parameter ρ for PICS and the smoothing parameter τ for SSF. In SSF this dependence is monotonous, whereas we cannot see a clear trend for ρ in PICS.

7. CONCLUSIONS

Hybrid dynamic parameter estimation problems can be solved successfully using reformulation methods. However, the parameters controlling the performance of the switching transition in the reformulated problem, i.e. ρ and τ for the penalization of the incomplete switching method and the smoothened step function approach, respectively, must be chosen with care. Both reformulation methods considered here proved to be quite robust against error in measurement.

8. ACKNOWLEDGEMENT

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