Model reduction for process control using iterative nonlinear identification

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***Abstract*— Given a complex first principles model of a process, a strategy for model complexity reduction is developed, such that the model obtained is suitable for process control. The system is assumed to have a Volterra representation that can be parametrized in terms of basis functions with fixed poles. The approach taken consists on iteratively using system identification techniques on the complex system model, while at the same time optimizing the inputs used. The results are tested on a copolymerization reactor example.**

Keywords: System identification, Volterra systems, input optimization, generalized basis functions, copolymerization.

I. Introduction

Detailed models for simulation purposes are often required in the process sector. They are usually based on first principles from physical and/or chemical considerations [1]. Once reliable parameters have been obtained, they have good prediction capabilities. However, they tend to be too complex for advanced process controller design, mainly because they are not explicitly developed for this purpose. On the other hand, simple models adequate for this may be developed, but they tend to be too simplistic, not capturing the complex process behavior correctly enough.

Given a simulation model for the process, this paper proposes a procedure for reducing its complexity to obtain a model that is simple enough to be used in process controller design, yet still captures the complex behavior of the system. The procedure combines several black-box empirical modeling techniques [2], [3], [4] with a certain knowledge of the plant. This allows to iteratively obtain a model using dedicated and optimized "experiments" to extract as much information as possible, based on the gained knowledge of the plant at each step. This might be unthinkable in the usual identification setting, where the number of experiments is a main limitation and furthermore signals are usually corrupted by noise.

The study is limited to systems admitting a Volterra representation [5], which is a rather general system class that fits the input/output behavior of many system processes. Furthermore, model based controllers can easily be designed based on this representation [6].

The procedure for complexity reduction combines frequency domain identification in the presence of nonlinearities [4], the use of generalized orthonormal bases for system representation [7], and forward selection orthogonal least squares methods [8], [9]. Additionally, the procedure is iterative, selecting both a set of candidate poles for the bases as in [10] and optimizing the input for invalidation of the current model during each iteration.

The next section reviews the discrete Volterra representation and its parametrization with respect to orthonormal basis functions. Section III gives an overview of the linear and nonlinear identification tools used, namely frequency domain identification and orthogonal least squares techniques. The complexity reduction procedure, together with some of its practical aspects is presented in Section IV. It is illustrated on the model of an exothermic copolymerization reactor in Section V. Finally, some conclusions are given. Throughout the text, $\mathbb{R}$ and $\mathbb{C}$ denote the real and complex sets, respectively, $\langle \cdot, \cdot \rangle$ denotes scalar product, $\overline{\xi}$ denotes the complex conjugate of ξ, sets are denoted with "blackboard bold" font, e.g. $\mathbb{X}$ or $\mathbb{Z}$, while vectors and matrices are denoted using boldface, e.g. $\boldsymbol{y}$ or $\boldsymbol{\Phi}$.

II. Process assumptions

The aim is to obtain a (possibly nonlinear) model $\mathcal{M}$ that is useful for process control design and satisfies

$$\hat{y}(t) = \mathcal{M}[u(t)] \approx \mathcal{S}[u(t)] = y(t). \tag{1}$$

This paper considers that $\mathcal{M}$ is discrete and, without loss of generality, $t \in \mathbb{N}$ is taken as normalized discrete time, i.e. $t = \tau/T_s$, where T_s is the sampling period and τ is physical time.

The input/output behavior of most control systems can be sufficiently well approximated by a Volterra series [11]. For SISO systems the finite memory Volterra system representation is given by [6]

$$\hat{y}(t) = y_0 + \sum_{j=1}^{n} v_M^j(t), \tag{2}$$

with $v_M^j(t) = v_k^j\left(u(t-1), \ldots, u(t-M)\right)$ the j-th order terms with memory length M, i.e.

$$v_M^j(t) = \sum_{i_1=0}^{M} \cdots \sum_{i_j=0}^{M} h(i_1, \ldots, i_j) \prod_{s=1}^{j} u(t-i_s). \tag{3}$$

It is a well known fact that *fading memory systems* [12] may be approximated uniformly on bounded input sets by a finite Volterra system with n and M sufficiently large. Finite Volterra models are BIBO stable, have periodic responses

to periodic inputs without subharmonic generation, and can exhibit input multiplicities, but no output multiplicities. They also preserve asymptotic constancy, i.e. if $u(t) \to u_s$ as $t \to \infty$, then $y(t)$ also approaches a constant limit y_s.

If the memory M is allowed to be infinite, then more complex nonlinear behaviors may be achieved. Furthermore, a very convenient parametrization in terms of *generalized orthonormal basis functions* (GOBFs) [13] may be possible. Given a set of poles $\{\xi_1, \xi_2, \dots, \}$ satisfying

$$\sum_{k=0}^{\infty} (1 - |\xi_k|) = \infty, \qquad |\xi_k| < 1, \\ \xi_k \in \mathbb{C} \implies \xi_{k+1} = \overline{\xi_k}, \tag{4}$$

the k-th GOBF is given by

$$B_k(z) = \frac{\sqrt{1-|\xi_k|^2}}{z - \xi_k} \prod_{i=1}^{k-1} \frac{1 - \overline{\xi}_i z}{z - \xi_i}. \tag{5}$$

The basis $\{B_1(z), B_2(z), \dots\}$ is complete in the Hardy space of functions analytic outside, and square integrable inside the unit circle, and the GOBFs are orthonormal, i.e. $\langle B_i, B_i \rangle = 1$ and

$$\langle B_i, B_j \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} B_i(e^{j\omega}) \overline{B_j(e^{j\omega})} d\omega = 0, \quad i \neq j. \tag{6}$$

These basis functions generalize the Laguerre basis ($\xi_k = \alpha$ for all k), the Kautz basis ($\xi_k = \gamma \exp(j\phi)$ for $k = 1, 3, \dots$) and the finite impulse response basis ($\xi_k = 0$).

If the Volterra kernels $h(\cdot)$ vary regularly with respect to $(i_1, \dots, i_j)$, they can be expanded using a generalized orthonormal basis as

$$h(i_1, \dots, i_j) = \sum_{r_1=1}^{\infty} \cdots \sum_{r_j=1}^{\infty} \gamma(r_1, \dots, r_j) \prod_{k=1}^{j} b_{r_k}(i_k). \tag{7}$$

where $b_r(t)$ is the inverse z-transform of $B_r(z)$, i.e.

$$b_r(t) = \mathcal{Z}^{-1} \{B_r(z)\}. \tag{8}$$

This expansion is exact if the kernels $h(\cdot)$ are *stably separable* and *strictly proper* [14], which basically means that high order kernels can be expressed as linear combinations of products of first order kernels and $h(i_1, \dots, i_j) = 0$ for $i_1 \cdots i_j = 0$. Substituting (7) in (3) and regrouping leads to

$$v_{\infty}^{j}(t) = \sum_{r_1=1}^{\infty} \cdots \sum_{r_j=1}^{\infty} \gamma(r_1, \dots, r_j) \prod_{k=1}^{j} \psi_{r_k}(t) \tag{9}$$

where

$$\psi_{r_k}(t) = \sum_{i=0}^{\infty} b_{r_k}(i) u_k(t-i). \tag{10}$$

Notice that (10) corresponds to the output of the GOBF $B_{r_k}(z)$ to the input $u(t)$. To get a finite dimensional model the infinite sums in (9) must be truncated and only the first q basis functions kept. Furthermore, since the products are commutative, several terms can be combined to obtain the more compact representation

$$\hat{y}(t) = y_0 + \sum_{j=1}^{n} \sum_{i_1=1}^{q} \cdots \sum_{i_j=i_{j-1}}^{q} \theta_{i_1,\dots,i_j} \prod_{k=1}^{j} \psi_{i_k}(t), \tag{11}$$

with the θ coefficients being linear combinations of γ terms. Knowing the GOBF's it is easy to identify the parameters, since they enter linearly, while the signals $\psi_i(t)$ are the responses of linear filters and therefore can be easily constructed. Note that (11) is nothing but a polynomial function $\pi : \mathbb{R}^q \to \mathbb{R}$ whose argument is the vector of filter outputs $\boldsymbol{\psi}(t)$, i.e.

$$\hat{y}(t) = \pi(\boldsymbol{\psi}(t)), \qquad \boldsymbol{\psi}(t) = \left[\psi_1(t), \dots, \psi_q(t)\right]^T. \tag{12}$$

Compared to the finite Volterra series (2), this parametrization usually requires only $q \ll M$ basis functions for comparable accuracy. For linear systems choosing poles close to the dominating frequencies permits a more compact representation [15]. A special emphasis is therefore put in the procedure for adequately selecting these poles.

III. Tools from system identification

Two identification techniques are used in the iterative procedure presented in Section IV: identification of a *best linear* system in the frequency domain (see **Step 1**) and forward selection using orthogonal least squares methods (see **Step 3**). The former is used to select a set of candidate poles to later build the GOBFs, while the latter is used for structure selection and parameter estimation.

Consider as excitation signal a *random multisine*, i.e. a periodic signal with fixed amplitude spectrum, but random phase spectrum. Let $U(k)$ and $Y(k)$ be, respectively, the measured input and output spectra with k the index for the excited frequency line. Under the Volterra representation assumption considered, the measured frequency response function (FRF) $Y(k)/U(k)$ will have the following decomposition under ideal measurements [16]:

$$G(j\omega_k) = G_0(j\omega_k) + G_B(j\omega_k) + G_S(j\omega_k). \tag{13}$$

$G_0(j\omega_k)$ corresponds to the underlying linear system and is independent of the input signal spectrum and $G_B(j\omega_k)$ is the *systematic* nonlinear contribution, which depends on the (deterministic) amplitude spectrum but not on the random phases. The *stochastic* nonlinear contributions $G_S(j\omega_k)$ are such that $Y_S(k) = G_S(j\omega_k)U(k)$ behaves like noise, uncorrelated with the input and with zero mean. Therefore, the response of the nonlinear system (2) to a random multisine can be regarded as the response through a *related linear dynamical system* $G_R(j\omega_k) = G_0(j\omega_k) + G_B(j\omega_k)$ plus some *nonlinear noise* due to the stochastic contributions.

From the many available techniques for system identification in the frequency domain (see [4] and the references therein), *subspace algorithms* [17] seem to be more adequate for the proposed approach. They produce a state space realization $(\hat{\boldsymbol{A}}, \hat{\boldsymbol{B}}, \hat{\boldsymbol{C}}, \hat{\boldsymbol{D}})$ for the fit $\hat{G}(z)$ to the FRF

$G(j\omega_k)$. A consistent estimate of $G_R(j\omega_k)$ with respect to the nonlinear noise is guaranteed as the number of realizations of the same random multisine tends to infinity, while the dynamic order must not be fixed *a priori*. This is important in the case studied, because the eigenvalues of $\hat{\boldsymbol{A}}$ constitute the significant candidate poles that will be tested later in the procedure.

Although (11) is linear in parameters, it is clear that even for a relatively small q, the number P of parameters can become quite large, namely $P = \binom{n+q}{q}$, so a structure selection is desirable. Note that (12) can be written as

$$y(t) = \boldsymbol{\varphi}^T(t)\boldsymbol{\theta} + e(t) \tag{14}$$

where $\boldsymbol{\theta} \in \mathbb{R}^P$ is the parameter vector, $\boldsymbol{\varphi} \in \mathbb{R}^P$ is the *regressor* vector, and $e(t)$ stands for the modeling error. Note that regressors $\varphi_j(t)$ are actually products of the outputs $\psi_i(t)$ from the GOBF filters (see (10) and (11)). The aim of structure selection is to keep only a reduced number of significant regressors. Forward selection schemes using orthogonal least squares techniques may be suitable to accomplish this task [9].

Given N time domain samples of the output

$$\boldsymbol{y} = \begin{bmatrix} y(1), & y(2), & \ldots, & y(N) \end{bmatrix}^T, \tag{15}$$

equation (14) can be written as

$$\boldsymbol{y} = \boldsymbol{\Phi}\boldsymbol{\theta} + \boldsymbol{e} = \boldsymbol{W}\boldsymbol{g} + \boldsymbol{e} \tag{16}$$

where the t-th row of the $N \times P$ matrix $\boldsymbol{\Phi}$ corresponds to the regressor $\boldsymbol{\varphi}^T(t)$. Furthermore it has been assumed that the matrix $\boldsymbol{\Phi}$ is decomposed as

$$\boldsymbol{\Phi} = \boldsymbol{W}\boldsymbol{R}, \qquad \boldsymbol{g} = \boldsymbol{R}\boldsymbol{\theta} \tag{17}$$

where $\boldsymbol{R} \in \mathbb{R}^{P\times P}$ is an upper triangular matrix and $\boldsymbol{W} = [\boldsymbol{w}_1, \ldots, \boldsymbol{w}_P]$ is a matrix with orthogonal columns. It is quite easy to see that the least squares solution $\hat{\boldsymbol{g}}$ to (16) satisfies $\hat{g}_i = \boldsymbol{w}_i^T\boldsymbol{y}/\boldsymbol{w}_i^T\boldsymbol{w}_i$ and furthermore each orthogonal regressor contributes independently to reducing the quadratic cost function $\boldsymbol{e}^T\boldsymbol{e}/\boldsymbol{y}^T\boldsymbol{y}$ with $\boldsymbol{e} = \boldsymbol{y} - \hat{\boldsymbol{y}}$, i.e.

$$J = \frac{\boldsymbol{e}^T\boldsymbol{e}}{\boldsymbol{y}^T\boldsymbol{y}} = 1 - \sum_{i=1}^{P} \frac{\boldsymbol{w}_i^T\boldsymbol{w}_i}{\boldsymbol{y}^T\boldsymbol{y}}\hat{g}_i^2. \tag{18}$$

By assuming that originally the columns of $\boldsymbol{\Phi}$ had been permuted such that the first ρ columns correspond to the most significant regressors in this sense, a reduced model is given by

$$\hat{\boldsymbol{y}} = \widetilde{\boldsymbol{W}}\tilde{\boldsymbol{\vartheta}} \qquad \text{and} \qquad \tilde{\boldsymbol{\vartheta}} = \widetilde{\boldsymbol{R}}\tilde{\boldsymbol{\theta}} \tag{19}$$

where $\widetilde{\boldsymbol{W}}$ comprises the first ρ columns of $\boldsymbol{W}$ and $\widetilde{\boldsymbol{R}}$ is defined accordingly. Orthogonal least squares forward selection is accomplished by performing the orthogonalization and the implicit column permutations of $\boldsymbol{\Phi}$ step by step. There are different techniques and selection criteria available [8]. For example, the D-LROLS algorithm [9] combines the modified Gram-Schmidt procedure with local regularization and a D-optimality design.

IV. Procedure for complexity reduction

The proposed methodology consists of two nested iteration loops. The outer loop proposes a set of candidate poles for a generalized orthonormal basis function (GOBF) parametrization of the Volterra representation, while the inner loop is used to select amongst the candidate poles only those which contribute significantly to improving the model, while at the same time selecting a sparse model structure.

Let the model at iteration κ be represented by $\mathcal{M}^{(\kappa)}$. The outer loop starts with $\kappa = 1$, a nonlinear model $\mathcal{M}^{(0)} = 0$, an empty set of GOBF poles $\mathbb{X}^{(0)} = \emptyset$, and an infinite cost $J^{(0)} = \infty$ (iterations are denoted by parenthesized indices). Consider the error system to be $\mathcal{E} = \mathcal{S} - \mathcal{M}^{(\kappa-1)}$.

Step 1. Fit a linear system $\widehat{G}_{\mathcal{E}}(z)$ to the measured frequency response function $G_{\mathcal{E}}(j\omega_k)$ of the error system $\mathcal{E}$. Collect its poles in the set $\mathbb{Z}^{(\kappa)} = \{\zeta_1, \ldots, \zeta_r\}$.

Step 2. Design an optimized control relevant input $u^{(\kappa)}(t)$, which tries to *invalidate* the current model $\mathcal{M}^{(\kappa-1)}$ with respect to $\mathcal{S}$ and obtain the output signal $y^{(\kappa)}(t) = \mathcal{S}[u^{(\kappa)}(t)]$. Up to here there also exists a set of *selected* GOBF poles $\mathbb{X}^{(\kappa-1)} = \{\xi_1, \ldots, \xi_q\}$.

Step 3. Sequentially modify the set $\mathbb{X}$ by adding one of the candidate poles $\zeta_j \in \mathbb{Z}$ at a time and building new models $\mathcal{M}$ until no significant increase in performance is noticed. After this step the set $\mathbb{X}^{(\kappa)}$ has been redefined, a new model $\mathcal{M}^{(\kappa)}$ has been obtained, and there is a cost $J^{(\kappa)}$ associated with it.

Step 4. If the new model has $J^{(\kappa)} \geq J^{(\kappa-1)}$ or $\mathcal{M}^{(\kappa)} \equiv \mathcal{M}^{(\kappa-1)}$, then **stop**. Otherwise, either repeat **Step 3** with other design criteria, e.g. a higher nonlinear degree, or repeat from **Step 1**, i.e. try to add more basis functions.

The inner loop concerns **Step 3** of the outer loop and starts defining $\mathbb{Z} = \mathbb{Z}^{(\kappa)}$, $\mathbb{X}_k = \mathbb{X}_k^{(\kappa-1)}$, and $J_{\min} = J^{(\kappa-1)}$, and generating $\boldsymbol{\psi}(t)$ as in (12) for the given input $u(t)$. The basic idea at each iteration is to build r candidate models $\mathcal{M}_j$, $j = 1, \ldots, r$ by considering that $\mathbb{X} = \{\xi_1, \ldots, \xi_q\}$ is augmented with the candidate pole ζ_j and then selecting one of these models. It consists of the following steps.

Step 3a (data generation). For each pole $\zeta_j \in \mathbb{Z}$, $j = 1, \ldots, r$, build

$$B_j(z) = \frac{\sqrt{1-|\zeta_j|^2}}{z-\zeta_j}\prod_{k=1}^{q}\frac{1-\overline{\xi_k}z}{z-\xi_k}. \tag{20}$$

Then generate outputs $\eta_j(t)$ as responses of $B_j(z)$ to the input $u_k(t)$ (see (10)), and build $\boldsymbol{\psi}_j(t) = \begin{bmatrix}\boldsymbol{\psi}^T(t), \eta_j(t)\end{bmatrix}^T$.

Step 3b (structure selection) Use each data pair $\big(\boldsymbol{\psi}_j(t), y(t)\big)$ to select a sparse model $\mathcal{M}_j$, e.g. using the D-LROLS algorithm [9], together with a corresponding performance index J_j.

Step 3c (pole selection). If $J_{j^*} < J_{\min}$ with $j^* = \arg\min J_j$ then redefine $\mathbb{X}$ and $\boldsymbol{\psi}(t)$ as $\mathbb{X} \cup \{\zeta_{j^*}\}$ and $\boldsymbol{\psi}_{j^*}(t)$ respectively. Furthermore define $J_{\min} = J_{j^*}$, and $\mathcal{M}^* = \mathcal{M}_{j^*}$ and return to **Step 3a** to test whether another candidate pole should be included. On the other hand, if

$J_{j^*} \geq J_{\min}$ then end this loop by defining $\mathbb{X}^{(\kappa)} = \mathbb{X}$, $\mathcal{M}^{(\kappa)} = \mathcal{M}^*$, and $J^{(\kappa)} = J_{\min}$.

In the following, the previous steps will be explained with more detail. Given a model $\mathcal{M}^{(\kappa-1)}$ and the complex simulation model $\mathcal{S}$ an error system $\mathcal{E}^{(\kappa)}$ can be defined, such that its output $e^{(\kappa)}(t)$ for some input function $\bar{u}^{(\kappa)}(t)$ is given by

$$e^{(\kappa)}(t) = \mathcal{E}^{(\kappa)}[\bar{u}^{(\kappa)}(t)] = \mathcal{S}[\bar{u}^{(\kappa)}(t)] - \mathcal{M}^{(\kappa-1)}[\bar{u}^{(\kappa)}(t)]. \tag{21}$$

Since the system $\mathcal{S}$ is assumed to have a Volterra representation, then so does the error system $\mathcal{E}^{(\kappa)}$ because $\mathcal{M}^{(\kappa-1)}$ is a Volterra model. Therefore the result (13) can be applied to find the best linear approximation during **Step 1**. The input $\bar{u}^{(\kappa)}(t)$ is thus designed as a random multisine with odd frequency components in order to minimize the effect of even nonlinearities when measuring the FRF [16]. The effect of the "nonlinear noise" can be attenuated by averaging over several realizations of $\bar{u}^{(\kappa)}(t)$. The subspace algorithm [17] uses this FRF frequency domain data to generate a state space realization, from which the candidate poles in $\mathbb{Z}^{(\kappa)}$ are obtained as the eigenvalues of the dynamic matrix $\hat{\boldsymbol{A}}$.

Once a set of candidate poles has been determined, an important feature of the procedure is designing the input $u^{(\kappa)}(t)$ to be used in the next structure identification and pole selection procedure. Assume that the previous model $\mathcal{M}^{(\kappa-1)}$ is the best possible sparse model for a GOBF-Volterra structure using a certain set $\mathbb{X}^{(\kappa-1)}$ of basis functions. If the complex system $\mathcal{S}$ can truly be represented by a GOBF-Volterra structure (2) with (9), then the error system $\mathcal{E}^{(\kappa)}$ would comprise the remaining terms that are not explicitly considered in $\mathcal{M}^{(\kappa-1)}$. This error system is precisely what is identified during **Step 3**, so an input signal that is adequate for this purpose is needed. This is done by invalidating the current model to uncover as much unmodeled dynamics as possible. The input is therefore chosen as that which *maximizes* the output of such an error system. Multisines are again considered, given their reported success for nonlinear Volterra system identification [18].

Assume a frequency grid with F lines has been chosen. Then the input signal $u(t)$ can be parametrized by its (complex) input spectrum $U(k)$. The optimization problem to solve is

$$U^*(k) = \arg\sup_{U(k)\in\mathbb{U}} \left\| \left(\mathcal{S} - \mathcal{M}^{(\kappa-1)} \right) [u(t)] \right\|^2 \tag{22}$$

whereby $\mathbb{U}$ refers to the set where the input spectrum is to be constrained and $\|\cdot\|$ is some norm. To solve this constrained optimization problem only a finite number of elements in the set $\mathbb{U}$ is considered and the $\sup$-operator is replaced by a $\max$-operator. Note, however, that this may not be an easy task and may prove to be time consuming.

Given some $\mathbb{X}$ and the input function $u^{(\kappa)}(t)$, it is not difficult to obtain the filter outputs $\boldsymbol{\psi}(t)$ by simulation. The same happens for obtaining $\eta_j(t)$ for each candidate GOBF filter $B_j(z)$ for each pole in $\mathbb{Z}$. For N samples the output vector $\boldsymbol{y}$ and r regressor matrices $\boldsymbol{\Phi}_j$ are built as in (15).

There are many reported techniques for structure selection [19]. Some stem from regression analysis, while others are based on more practical aspects. When the number of candidate regressors is large, as will be usual in this case, forward selection schemes appear to be more adequate. The orthogonal least squares techniques can be combined with an information criterion to stop adding regressors to the structure, e.g. Akaike's well known criterion (AIC) [20].

Least squares methods deliver unbiased model estimates if the considered structure corresponds to the true system structure up to some normally distributed error with certain statistical properties. However, this is often not the case when identifying nonlinear models, so in the end the obtained model might indeed conform very well to the particular data set with which it was obtained, but not to other distinct data. Given the possibility of simulation, the structure selection and parameter estimation carried on during **Step 3b** of the procedure can be reinforced with cross-validation with other data sets.

It has been observed that forward selection techniques tend to include spurious regressors [21]. It is likely that if instead of just one data set $(\boldsymbol{\Phi}, \boldsymbol{y})$, several data sets are available, say $(\boldsymbol{\Phi}_\ell, \boldsymbol{y}_\ell)$ for $\ell = 1, \ldots, L$, then the structure selection procedure can be made more efficient. A simplistic way of doing this is to keep only those regressors that repeat themselves on the identified structures corresponding to each data set. Another way is to test whether two regression equations are statistically equal by testing the hypothesis that some of the corresponding regressor coefficients are the same for both data sets.

V. Example

The procedure is illustrated on the model of a continuous copolymerization reactor with exothermic kinetics. The model has 15 states, 6 inputs $\boldsymbol{u}$, and 7 outputs $\boldsymbol{y}$ [22]. The inputs are the feed rates of the two monomers vinyl acetate (u_1) and methyl-methacrylate (MMA) (u_2), the transfer agent acetaldehyde (u_3), and the inhibitor m-dinitrobenzene (u_4), plus the coolant (u_5) and feed (u_6) temperatures. The outputs are the effluent compositions of the two monomers and the solvent (benzene) in the separator (y_1-y_3), the reactor temperature (y_4), the polymer production rate (y_5) the copolymer composition (y_6), and its intrinsic viscosity (y_7). The main nonlinearity of the system is due to the temperature dependent kinetics of Arrhenius type.

Although the system is MIMO, to consider it as a SISO system, it was initially set to the operating conditions

$$\boldsymbol{u}_s = \left[3, 0.3, 0.25, 0.01, 373, 353\right]^T,$$
$$\boldsymbol{y}_s = \left[0.1455, 7.786, 1.8219, 380, 0.412, 0.543, 27.1\right]^T.$$

and then only one input/output pair was considered. That is, only one input was made time-varying, while the others

were kept at their operating condition values $\boldsymbol{u}_s$. Just one output was observed. The rates u_1-u_4 and y_5 are given in [kg/min], temperatures u_5,u_6 and y_4 are given in [K], effluent compositions y_1-y_3 in [kmol/m^3], intrinsic viscosity in [l/kg] and the copolymer composition is dimensionless.

For illustration purposes the input/output pairs (u_2, y_7) and (u_4, y_5) were considered because previous testing detected the most sensitivity with these pairs. In both cases structure selection was enhanced by considering several data sets.

For the pair (u_2, u_7) the sampling time was set to $T_s = 10$ [min] and input deviations of $\pm 50\%$ from $u_{2,s} = 0.3$ [kg/min] were used. Prior to **Step 1** a maximal frequency $f_{\max} = 256 f_0$ for the multisines was first experimentally determined to avoid aliasing due to harmonic generation and afterwards $F = 256$ frequency lines were always used. The procedure was tested several times and consistently after only two iterations a model with only 4 real poles was obtained. These were, for example:

$$\mathbb{X} = \{0.9598, 0.8483, 0.8613, 0.9641\}. \tag{23}$$

The resulting model had the quadratic structure

$$\hat{y}(t) = \boldsymbol{\psi}^T(t)\boldsymbol{\theta} = \begin{bmatrix} \psi_1(t) \\ \psi_2(t) \\ \psi_1(t)\psi_3(t) \\ \psi_2^2(t) \\ \psi_2(t)\psi_4(t) \\ \psi_3^2(t) \\ \psi_4^2(t) \end{bmatrix}^T \begin{bmatrix} 5.8209 \\ 2.7152 \\ -2.2462 \\ 1.1000 \\ -1.4406 \\ 2.2384 \\ 0.6363 \end{bmatrix} \tag{24}$$

with $\psi_i(t)$ the output of the corresponding GOBF. After identification, the model was tested on a completely different validation input, namely a random step input [23]. The output of both the complex simulation model and the model (24) is shown in Fig. 1, together with the percentage deviation error and the input used.

For the input/output pair (u_4, y_5) the sampling time was set to $T_s = 1$ [min] and input deviations of ± 15 [K] from $u_{4,s} = 373$ [K] were used. Again the procedure was tested several times and again two iterations were enough to obtain a satisfactory model. The following 3 GOBF poles were obtained:

$$\mathbb{X} = \{0.9152 \pm j0.0271, 0.8832\}, \tag{25}$$

and the model resulted with the following cubic structure:

$$\hat{y}(t) = \begin{bmatrix} \psi_1(t) \\ \psi_2(t) \\ \psi_3(t) \\ \psi_1^2(t) \\ \psi_1(t)\psi_2(t) \\ \psi_2^2(t) \\ \psi_2(t)\psi_3(t) \\ \psi_3^2(t) \\ \psi_2^3(t) \\ \psi_2(t)\psi_3^2(t) \end{bmatrix}^T \begin{bmatrix} 2.5679 \times 10^{-3} \\ 0.2685 \times 10^{-3} \\ 0.0567 \times 10^{-3} \\ 4.5304 \times 10^{-6} \\ -13.636 \times 10^{-6} \\ -5.3173 \times 10^{-6} \\ 10.462 \times 10^{-6} \\ 2.3806 \times 10^{-6} \\ 0.0681 \times 10^{-6} \\ -0.0166 \times 10^{-6} \end{bmatrix} \tag{26}$$

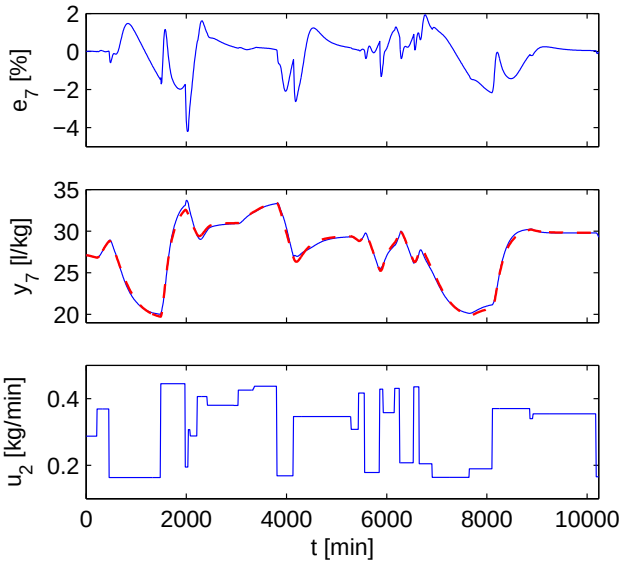

Fig. 1. I/O pair (u_2, y_7). **Top:** modeling error. **Middle:** outputs of complex simulation model (dashed) and reduced complexity model (solid). **Bottom:** random step input.

with $\psi_i(t)$ the output of the corresponding GOBF. This model was tested on a random step input and the results are shown in Fig. 2,

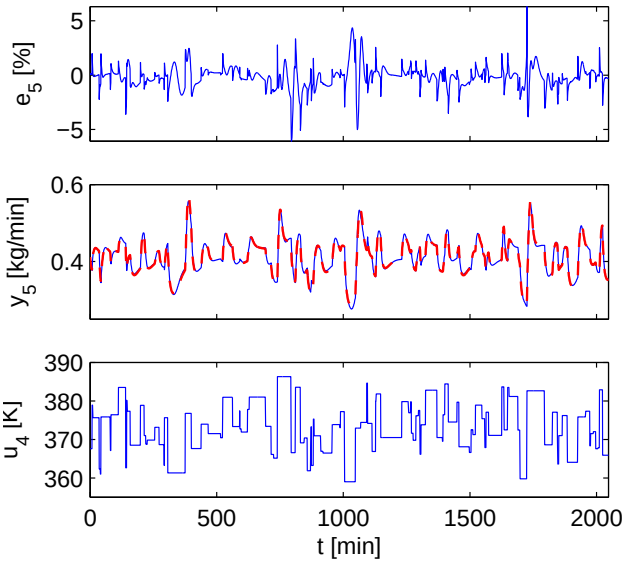

Fig. 2. I/O pair (u_4, y_5). **Top:** modeling error. **Middle:** outputs of complex simulation model (dashed) and reduced complexity model (solid). **Bottom:** random step input.

VI. Conclusions

A procedure for complexity reduction combining frequency domain linear identification, constrained input optimization techniques, and substructure selection and parameter estimation methods has been proposed. Testing the procedure on a realistic example shows promising results

and further investigations are under way to refine it and extend it to MIMO systems, as well as testing it on more complex nonlinear systems.

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