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Bilinear approach employed for modelling of continuous stirred tank reactor processes

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***Abstract*—In this paper feasibility of modelling approach based on a bilinear system approximation is demonstrated on one of the most frequently met processes in chemical engineering, namely a continuous stirred tank reactor. Selected examples of such systems from the literature are considered and modelled with a use of dynamic bilinear systems. Advantages of this approach are presented and discussed.**

I. Introduction

Chemical reactor is often described as 'the most important unit operation in a chemical process', see [1]. The task of its modelling and control is commonly encountered in the literature representing a practical nonlinear industrial problem, see [2], [3], [4]. A popular model of a chemical reactor is the so-called continuous stirred tank reactor (CSTR). CSTR consists of a closed tank to which an input stream is fed in and the output stream fed out in a continuous manner, whilst a content is constantly stirred. Modelling of CSTRs is challenging mainly due to i) possibility of occurrences of rapid reactions (the so-called ignition-extinction phenomena), hence fast changing process gain and dynamics, and also due to ii) nonlinear steady-state behaviour, see [1] and [5].

This paper demonstrates that the CSTRs can be modelled by employing an approach based on bilinear system (BS) description. In order to increase modelling flexibility of BSs, an extension consisting of a static nonlinearity that transforms the input signal is proposed. Such a structure, referred to as a Hammerstein-bilinear system (HBS), see [6], [7], is considered and compared to BS and Hammerstein system (HS) models.

The use of BS based approach is motivated twofold. First, BSs retain a close structural relationship with linear models, hence standard well understood notions from classical linear system theory such as system time constants, damping/natural frequency and steady-state gain are to large extent retained. This follows from the property that BS structure can be interpreted as a linear time-varying system, which also greatly facilitates the control design. Second, BSs preserve linearity w.r.t. the parametrisation, which aids in their identification by allowing for standard parameter estimation methods to be used.

In this paper three different CSTR models are considered. Two of the models are isothermal, whilst the third model is an example of a diabatic CSTR, see [1].

II. Model structures

HBS structure belongs to a sub-class of so-called output affine models, i.e. models that retain affinity w.r.t. the output signals, see [8]. It comprises of a cascade connection of a static (memoryless) nonlinearity followed by a dynamic time-invariant affine BS and is given by

$$y_k = \sum_{j=1}^{n_a} a_j y_{k-j} + \sum_{i=1}^{n_b} b_i v_{k-i} + \sum_{j=1}^{n_a}\sum_{i=1}^{n_b} \eta_{ij} v_{k-i} y_{k-j} + c \quad (1)$$

$$v_k = f(u_k) \quad (2)$$

where a_j, b_i, η_{ij} and c are model parameters. The bilinearity is defined as a product between system output y_k and the intermediate input variable v_k, and $f(\cdot)$ denotes a general scalar static nonlinear function. Note that not all bilinear coefficients must necessarily be present in (1), hence a particular structure can be obtained by setting selected η_{ij} to zero.

The HBS can be interpreted as a generalisation of both of its constituent subsystems, i.e. HS and BS models. In particular, a BS is obtained from (1)-(2) by setting $u_k = v_k$, i.e. by selecting $f(x) = x$, which gives

$$y_k = \sum_{j=1}^{n_a} a_j y_{k-j} + \sum_{i=1}^{n_b} b_i u_{k-i} + \sum_{j=1}^{n_a}\sum_{i=1}^{n_b} \eta_{ij} u_{k-i} y_{k-j} + c \quad (3)$$

Similarly, a HS is obtained by setting $\eta_{ij} = 0 \; \forall \; i, j$ in (1)-(2), which leads to

$$y_k = \sum_{j=1}^{n_a} a_j y_{k-j} + \sum_{i=1}^{n_b} b_i v_{k-i} + c \quad (4)$$

$$v_k = f(u_k) \quad (5)$$

Also, a linear (or more precisely an affine) structure is obtained by imposing both restrictions simultaneously, i.e. $\eta_{ij} = 0 \; \forall i, j$ and $u_k = v_k$.

In this paper, for simplicity, it is assumed that the input static nonlinearity is modelled as a polynomial of order n_α, i.e.

$$f(x) = \sum_{l=1}^{n_\alpha} \alpha_l x^l \quad (6)$$

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Consequently, a particular HBS structure is given by a quadruplet that defines the number of a, b, η and α coefficients, i.e. HBS(n_a,n_b,n_η,n_α). Moreover, the sum of all coefficients plus unity (to account for an offset), corresponds to the total number of degrees of freedom (DoF) in a given structure. An analogous notation is used w.r.t. other structures that can be derived from the HBS model.

III. Parameter estimation

The HBS structure is bilinear in terms of parametrisation, due to the products between α and a, and also between α and η coefficients. A well known approach to solve such problems is to use the so-called bilinear parametrisation method (BPM), see [9]. The BPM solves the estimation problem in a two step manner, where in the first step α parameters are fixed and a, b, η parameters are calculated, whilst in the second step a, b and η remain fixed and α parameters are computed [10]. Because the two subproblems separately are linear w.r.t. the unknowns, the ordinary least squares algorithm [9] can be applied, which renders the overall procedure numerically efficient, and this is the approach used here. An analogous technique can also be applied to HS models, see [11], whilst the parameters of affine and BS structures can be estimated by using a single ordinary least squares technique.

IV. Simulation studies

A. Performance criteria and experimental setup

In order to quantify the accuracy of models obtained, two performance criteria are used. Namely, the coefficient of determination and the (normalised) integral of absolute error, defined, respectively, as follows

$$\mathrm{R}_\mathrm{T}^2 = 100\left(1 - \frac{\|y-\hat{y}\|_2^2}{\|y-\bar{y}\|_2^2}\right) \tag{7}$$

$$\mathrm{IAE} = \frac{1}{N}\sum_{k=1}^{N}|y_k - \hat{y}_k| \tag{8}$$

where y and $\hat{y}$ denote vectors composed of the measured (noisy) system outputs and outputs generated by the estimated model, respectively, and $\bar{y}$ is the mean value of y. The notation $\|\cdot\|_2$ denotes the Euclidean norm.

Because the main interest of experiments lies in the modelling capabilities of the model structures considered, relatively long input-output data consisting of $N = 20,000$ samples are used. Three data sets are considered, i.e. identification and two validation data sets. The sampling time is chosen as 0.1s. In the case of the identification data set and the first validation data set, the input signal is generated as a series of uniformly distributed steps between the minimal and maximal range for a given system. The probability of transition to a different level is selected randomly with a uniform switching probability of 10%, providing a reasonable compromise between the content of transient and steady-state data. Additionally, to ensure that the input is sufficiently exciting, a normally distributed, white and zero-mean noise sequence of comparatively small variance is added. To render the identification experiment more realistic, the measured output is assumed to be contaminated with an additive, normally distributed, white and zero-mean disturbances such that the resulting signal-to-noise ratio is approximately 37dB. The second validation data set comprises of a monotonic staircase input, which allows the performance of the identified models to be evaluated with the emphasis placed on the steady-state behaviour. Also, to provide an indication of the complexity of the models, the corresponding DoF are considered.

B. Isothermal CSTR with a first-order irreversible reaction

1) System description: The first isothermal CSTR model considered, referred to as the CSTR1, is given by the following equations, see [1] for details, i.e.

$$\frac{dC_A(t)}{dt} = \frac{F(t)}{V}C_{Af} - \left(\frac{F(t)}{V} + k\right)C_A(t) \tag{9}$$

$$\frac{dC_B(t)}{dt} = -\frac{F(t)}{V}C_B(t) + kC_A(t) \tag{10}$$

and describes a first-order irreversible reaction $A \xrightarrow{k} B$ where k is the reaction rate per unit volume. The remaining variables are: $C_A(t)$, $C_B(t)$ - concentrations of substances A and B inside the tank of a constant volume V, respectively, $F(t)$ - inflow/outflow mass rate, C_{Af} - inflow concentration of substance A. Only the substance A is present in the inflow stream, and inflow and outflow mass rates are equal. The actual units are unimportant and hence are not included. It is assumed that the manipulated variable is $F(t)$ and that $C_B(t)$ is the output of interest. The task consists of identifying a model between $F(t)$ and $C_B(t)$.

The values of the parameters were chosen as $V = 1$, $k = 0.2$, $C_{Af} = 1$ and the initial states of the process as $C_{a0} = C_{b0} = 0.5$, where the subscript zero denotes the initial value. The input $F(t)$ is in range of $(0,\ 1]$.

It is observed that a product, i.e. bilinearity, between the input $F(t)$ and the state $C_A(t)$ occurs in (9) and that an analogous product between the input $F(t)$ and the state $C_B(t)$ is also present in (10). The steady-state characteristic of the CSTR1 model is plotted in Figure 1, where it is observed that the curve resembles the type of steady-state characteristics typical of BSs. Therefore, these observations substantiate the usage of a bilinear based modelling approach.

2) Identification results: Selected identification results are given in Table I. First, it is observed that the model is considerably nonlinear because the third order affine structure resulted in R_T^2 below 90% for all three data sets. Further increase of the order of the affine structure does not lead to any significant improvements in modelling performance. HS models show clear improvement, allowing for R_T^2 of approximately 98% in the case of the HS(1,1,4) to be achieved for all three data sets. Further increase of the order of the input polynomial does not lead to significant improvements in model fitting. This is due to the fact that the nonlinear steady-state characteristic is not a complex function, and it is rather the changing system dynamics that is not captured by the HS type structures. When considering the results obtained from BS models, an evident

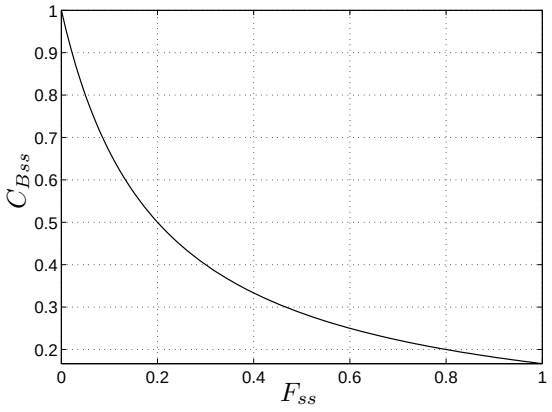

Fig. 1. CSTR1 - A steady-state characteristic.

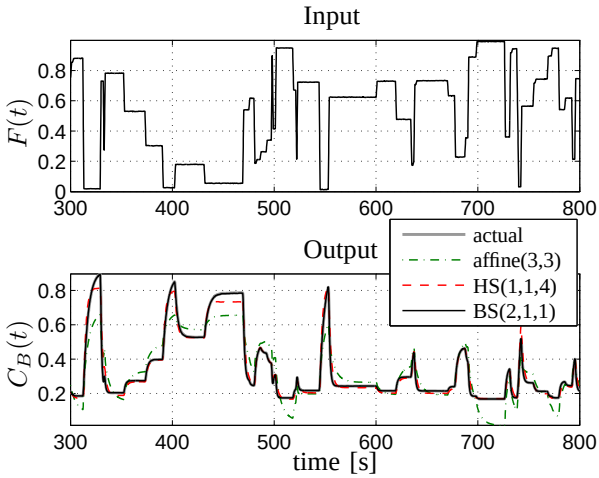

Fig. 2. CSTR1 - Selected representative results of identification on validation data set 1 in the interval $[300,\ 800]$s.

structure		Id. data set		Val. data set 1		Val. data set 2	
	DoF	R^2_T	IAE $\times 10^{-3}$	R^2_T	IAE $\times 10^{-3}$	R^2_T	IAE $\times 10^{-3}$
affine(3,3)	7	80.40	54.49	80.08	55.27	88.11	74.10
HS(1,1,2)	5	96.70	24.04	96.10	25.13	94.78	31.00
HS(1,1,3)	6	97.81	15.51	97.83	17.16	96.92	19.39
HS(1,1,4)	7	98.10	13.75	98.10	15.68	97.49	17.57
BS(1,1,1)	4	99.97	2.265	99.97	2.276	99.97	2.716
BS(2,1,1)	5	99.98	1.845	99.98	1.851	99.99	1.983
HBS(1,1,1,2)	6	99.97	2.275	99.97	2.304	99.97	2.748
HBS(1,1,1,3)	7	99.99	1.421	99.97	2.260	99.99	1.751

TABLE I
CSTR1 - QUANTIFIED IDENTIFICATION AND VALIDATION RESULTS FOR MODEL STRUCTURES CONSIDERED.

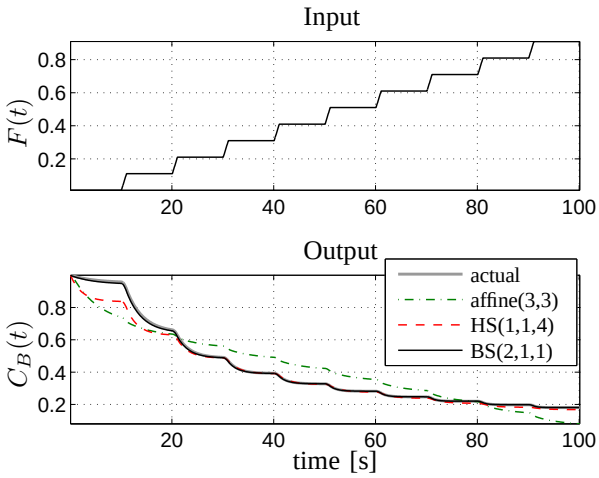

Fig. 3. CSTR1 - Selected results of identification on validation data set 2.

improvement in the approximation performance is noted, i.e. the R^2_T of almost 100% is obtained with the IAE criterion decreasing by approximately 7 times, when compared to the best HS model. This means that both, the nonlinear steady-state characteristic and the changing system dynamics are approximated well by the BS structures with only 4 or 5 DoF. Because the only source of nonlinearity in the underlying process equations arises from product terms, cf. (9)-(10), this result could have been anticipated.

Representative graphical results of the identification are given in Figures 2 and 3, showing the performances of the selected estimated models on arbitrarily chosen intervals of the validation data sets 1 and 2, respectively. It is observed that in the case of both figures the actual system output is virtually undistinguishable from that generated by the identified BS(2,1,1) structure. Consequently, it is concluded that a BS structures are appropriate for modelling the CSTR1 process.

C. Isothermal CSTR with the Van de Vusse reaction

1) System description: The second isothermal CSTR model considered, see [1], referred to as the CSTR2, is given by

$$\frac{dC_A(t)}{dt} = \frac{F(t)}{V}\big(C_{Af} - C_A(t)\big) - k_1 C_A(t) - k_3 C_A^2(t) \quad (11)$$

$$\frac{dC_B(t)}{dt} = -\frac{F(t)}{V} C_B(t) + k_1 C_A(t) + k_2 C_B(t) \quad (12)$$

$$\frac{dC_C(t)}{dt} = -\frac{F(t)}{V} C_C(t) + k_2 C_B(t) \quad (13)$$

$$\frac{dC_D(t)}{dt} = -\frac{F(t)}{V} C_D(t) + \frac{1}{2} k_3 C_A^2(t) \quad (14)$$

with the behaviour governed by the so-called Van de Vusse reaction kinetics. The reactions

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \quad (15)$$

$$2A \xrightarrow{k_3} D \quad (16)$$

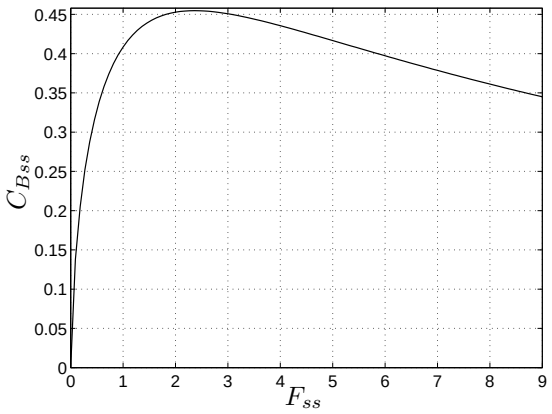

Fig. 4. CSTR2 - A steady-state characteristic.

structure		Id. data set		Val. data set 1		Val. data set 2	
	DoF	R^2_T	IAE $\times 10^{-3}$	R^2_T	IAE $\times 10^{-3}$	R^2_T	IAE $\times 10^{-3}$
affine(3,3)	7	10.92	44.68	7.724	46.06	5.539	54.19
HS(1,1,4)	7	84.07	15.67	84.03	16.86	89.50	25.10
HS(1,1,5)	8	91.48	10.70	91.16	12.38	94.40	16.13
HS(1,1,6)	9	94.99	8.552	94.56	8.803	97.32	11.28
HS(1,1,7)	10	96.43	6.591	96.09	6.800	98.61	8.118
HBS(1,1,1,3)	7	92.96	10.72	92.78	11.43	98.23	11.31
HBS(1,1,1,4)	8	98.11	4.335	98.11	4.726	99.86	3.000
HBS(1,1,1,5)	9	98.34	3.257	98.33	3.551	99.60	3.747

TABLE II
CSTR2 - QUANTIFIED IDENTIFICATION AND VALIDATION RESULTS FOR MODEL STRUCTURES CONSIDERED.

are irreversible and described by the reaction rate constants k_1, k_2 and k_3. The remaining variables are: $C_A(t)$, $C_B(t)$, $C_C(t)$, $C_D(t)$ - concentrations of substances A, B, C and D inside the tank of constant volume V, respectively, $F(t)$ - inflow/outflow mass rate, C_{Af} - inflow concentration of substance A. Only the substance A is present in the inflow stream, and inflow and outflow mass rates are equal. It is assumed that the manipulated variable is $F(t)$, whilst $C_B(t)$ is the output of interest. Therefore, the modelling task consists of identifying a model between $F(t)$ and $C_B(t)$.

The values of the parameters were chosen as: $V = 1$, $k_1 = 5/6$, $k_2 = 3$, $k_3 = 10/6$, $C_{Af} = 10$ and the initial states of the process are $C_{a0} = C_{b0} = 0$. The input $F(t)$ is postulated to vary between $(0, 9]$.

It is observed that a bilinearity between the input $F(t)$ and the state $C_A(t)$ is present in (11) and an analogous bilinearity between the input $F(t)$ and the state $C_B(t)$ appears in (12). However, in contrast to (9) corresponding to the CSTR1 model, here the product term is not the only source of nonlinearity in the evolution of $C_A(t)$. This is due to the presence of the expression $C_A^2(t)$ in (11), whose influence is controlled by the rate constant k_3.

Consequently, it is concluded that although the underlying system equations indicate that a bilinear type behaviour is present, it may be infeasible to model the process by a BS

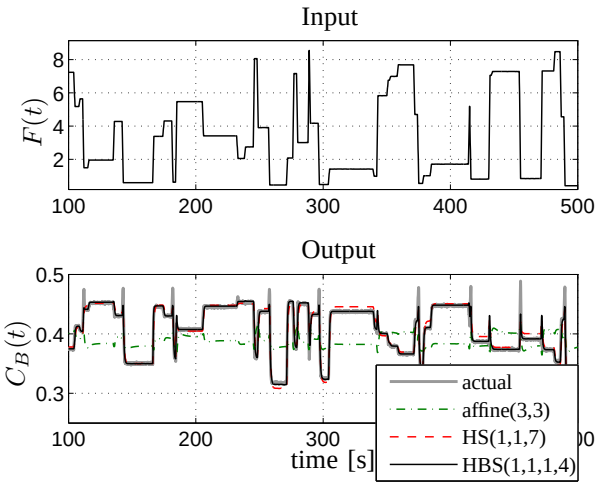

Fig. 5. CSTR2 - Selected representative results of identification on validation data set 1 in the interval $[100,\ 500]$s.

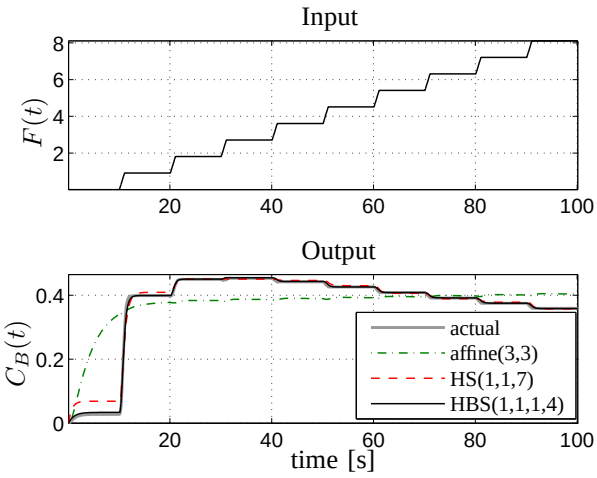

Fig. 6. CSTR2 - Selected results of identification on validation data set 2.

only over the entire range of its operation. This hypothesis is confirmed by considering the steady-state characteristic of the CSTR2 process given in Figure 4, where it is observed that the system exhibits the input multiplicity (IM) property [3]. Such static behaviour cannot be captured by a BS, due to its inherent structural limitations. This stands in contrast to HS and HBS that are structurally capable of IM, hence are anticipated to be more appropriate for modelling of the CSTR2 process.

2) Identification results: The identification results are given in Table II, where a low value of R^2_T for all three data sets in the case of the affine model indicates that the overall process is considerably nonlinear. Further increase of the order of the affine structure does not result in noticeable improvements in fitting. The performance criteria of BS structures are not included in the table because it was not possible to fit such models, i.e. the corresponding R^2_T values were negative. This result confirms the inappropriateness of using BS structures for approximating processes exhibiting IM. A considerable

improvement is achieved in the case of HS structures, when compared to the affine model, with R_T^2 of about 97% on average for all three data sets obtained by HS(1,1,7) with 10 DoF. The results obtained by the HBS(1,1,4) and HBS(1,1,5), with 8 and 9 DoF, respectively, show further fitting improvements with both models achieving R_T^2 of approximately 98% for the identification data set and the validation data set 1, and almost 100% for the validation data set 2. Compared to the HS(1,1,7) the IAE was reduced by approximately threefold in the case of the first two data sets, and fourfold in the case of the third data set.

Representative graphical results obtained from the identification procedure are presented in Figures 5 and 6, showing the performances of the selected estimated models on arbitrarily chosen intervals of the validation data set 1 and 2, respectively. Whilst in the case of Figure 5 slight discrepancies between the actual output and that generated by the estimated HBS(1,1,1,4) model are observed, the two corresponding curves are virtually indistinguishable in the case of Figure 6. Also, it is noted that the system exhibits a non-minimum phase behaviour when $F(t)$ is high and changes to a lower value. This behaviour, which is observed to be manifested by spikes in the $C_B(t)$ signal, increases the difficulty of obtaining an acceptable approximation. Consequently, despite such a challenging task, the modelling results obtained by the HBS(1,1,1,4) structure can be treated as very satisfactory in overall.

D. Diabatic CSTR

1) System description: The considered diabatic CSTR model, see [1] and [5], referred to as the CSTR3, is given by

$$\frac{dC_A(t)}{dt} = \frac{F(t)}{V}\big(C_{Af} - C_A(t)\big) - k_0 r(t) C_A(t) \tag{17}$$

$$\frac{dT(t)}{dt} = \frac{F(t)}{V}\big(T_f - T(t)\big) + \frac{-\Delta H}{\rho c_p} k_0 r(t) - \frac{US}{V\rho c_p}\big(T(t) - T_j(t)\big) \tag{18}$$

where the first order reaction rate per unit volume is given by the so-called Arrhenious expression, i.e.

$$r(t) = \exp\left(\frac{\Delta E}{RT(t)}\right) \tag{19}$$

The other variables are: $C_A(t)$ - concentration of substance A inside a tank of the constant volume V, $F(t)$ - inflow/outflow mass rate, C_{Af} - inflow concentration of substance A, k_0 - pre-exponential factor, R - ideal gas constant, ΔE - activation energy, $T(t)$ - reactor temperature, T_f - inflow (feed) temperature, $T_j(t)$ - jacket temperature, U - overall heat transfer coefficient, $-\Delta H$ - heat of reaction, ρ - density, S - area for heat exchange, c_p - heat capacity. Only the substance A is present in the inflow stream, and inflow and outflow mass rates are equal. It is assumed that the manipulated variable is $T_j(t)$, whilst $C_A(t)$ is the output of interest. Therefore, the modelling task consists of identifying a model between $T_j(t)$ and $C_A(t)$.

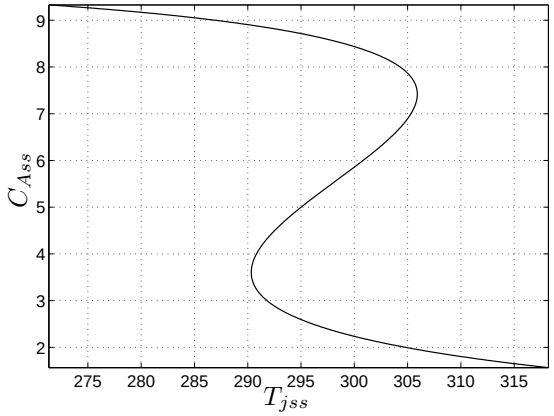

Fig. 7. CSTR3 - A steady-state characteristic.

structure		Id. data set		Val. data set 1		Val. data set 2	
	DoF	R_T^2	IAE $\times 10^{-3}$	R_T^2	IAE $\times 10^{-3}$	R_T^2	IAE $\times 10^{-3}$
affine(3,3)	7	88.86	99.53	88.84	99.38	90.73	96.42
HS(1,1,3)	6	96.92	49.26	96.88	49.52	96.65	54.41
HS(1,1,5)	8	97.31	45.51	97.30	45.63	97.20	49.03
HS(1,1,7)	10	97.89	39.41	97.86	39.74	98.00	40.15
HS(2,2,3)	8	97.19	45.61	97.15	45.88	98.46	40.48
HS(2,2,5)	10	97.61	41.52	97.57	41.80	98.79	36.90
HS(2,2,7)	12	98.16	35.46	98.12	35.77	99.16	31.27
BS(1,1,1)	4	98.98	27.52	98.96	27.09	99.20	23.82
BS(2,1,1)	5	98.90	28.35	98.88	28.75	99.14	25.08
BS(2,2,2)	7	99.16	23.35	99.13	23.90	99.58	16.72
HBS(1,1,1,3)	7	99.13	25.63	99.11	26.00	99.15	24.77
HBS(1,1,1,5)	9	99.19	24.61	99.18	24.98	99.21	23.58
HBS(1,1,1,7)	11	99.28	22.50	99.27	22.97	99.36	20.16
HBS(2,2,2,3)	10	99.39	20.96	99.37	21.40	99.52	18.68
HBS(2,2,2,5)	12	99.46	19.53	99.44	20.05	99.58	16.96
HBS(2,2,2,7)	14	99.56	17.25	99.54	17.84	99.70	13.52

TABLE III
CSTR3 - QUANTIFIED IDENTIFICATION AND VALIDATION RESULTS FOR MODEL STRUCTURES CONSIDERED.

Considering equations (17) and (18), it is noted that in each case bilinearities are present, i.e. products between $F(t)$ and the state $C_A(t)$ in the first equation and between $F(t)$ and the state $T(t)$ in the second equation. These, however, are clearly not the only contributions that render nonlinearity of the overall behaviour. This is due to the presence of nonlinear relationships involving an exponent of $T(t)$ that appear in both equations.

A steady-state characteristic of the CSTR3 model, given in Figure 7, shows the presence of the output multiplicity (OM) property [3]. Because non of the model structures investigated in this paper is structurally capable of OM, see [8], only a restricted range of the process operation is considered, i.e. the range of $T_j \in [273,\ 306)$ within which OM is absent. Consequently, because the operating range is limited, it might be possible that a bilinear type behaviour will, in fact, be prevailing.

The values of the parameters were chosen as: $F(t) = 1$,

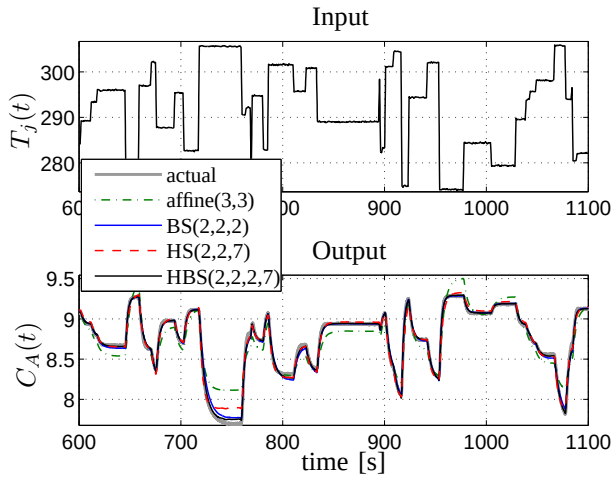

Fig. 8. CSTR3 - Selected representative results of identification on validation data set 1 in the interval $[600,\ 1100]$s.

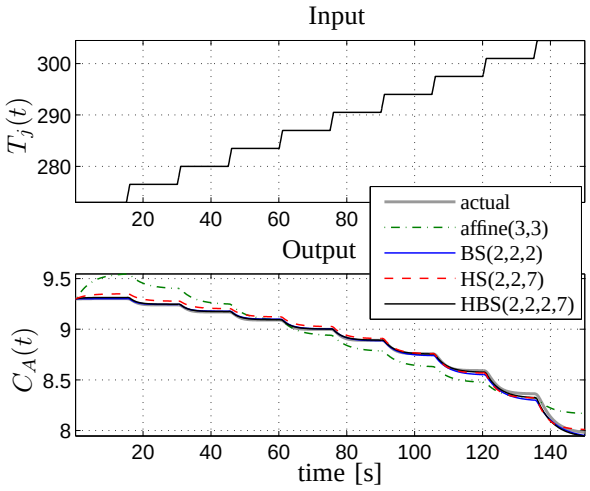

Fig. 9. CSTR3 - Selected results of identification on validation data set 2.

$V = 1$, $k_0 = 9703 \times 3600$, $-\Delta H = 5960$, $\rho c_p = 500$, $US = 150$, $\Delta E = 11843$, $R = 1.987$ and the initial states of the process are $C_{A0} = 8.5$ and $T_0 = 305$.

2) Identification results: The identification results obtained are collected in Table III, from where it is observed that the affine model achieved reasonable results close to 90% in terms of R_T^2 in the case of all three data sets. Further increase of the order of the affine structure does not provide any considerable improvements. First order HS structures yielded results that are better by approximately 8% on average in terms of the R_T^2 criterion and approximately twice on average in terms of the IAE criterion. This indicates a clear improvement and justifies the need for a nonlinear model structure. The best fitting among HS structures is obtained for a second order HS structure, i.e. HS(2,2,7) with a seventh order polynomial and 12 DoF in total. It is interesting to notice that these values are close to those produced by a relatively simple BS structure, i.e. BS(1,1,1), with only 4 DoF. A boundary of 99% in terms of the R_T^2 criterion is exceed by a second order BS model with 7 DoF. The fitting is improved, if at all, only slightly by first order HBS structures, and it is the second order HBS model, i.e. HBS(2,2,2,7), in the case of which the results improve more significantly. However, this comes at the cost of 14 DoF, when compared to only 7 DoF in the case of BS(2,2,2).

Representative graphical results generated from the estimated models are depicted in Figures 8 and 9, and demonstrate the performances of the selected models on arbitrarily chosen intervals of the validation data set 1 and 2, respectively. It is observed that the outputs of the estimated models BS(2,2,2) and HBS(2,2,2,7) are both virtually undistinguishable from the actual system output in both figures. Consequently, by taking into account the corresponding DoF and a pragmatic point of view, it is the second order BS that appears to be a preferable choice in this case.

V. Conclusions

The paper has demonstrated feasibility of BS based modelling approach for approximating CSTRs. It has been shown that BS models are capable of capturing both, i.e. the dynamic and static behaviour of the exemplary CSTR systems considered. In the case of the CSTR process exhibiting the IM property, a BS structure with an additional nonlinear memoryless element transforming the input, i.e. a HBS structure, has shown to be an appropriate choice.

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