

USING ARX APPROACH FOR MODELLING AND PREDICTION OF THE DYNAMICS OF A REACTOR-EXCHANGER

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The main aim of this paper is to establish a reliable model of a process under its normal operating conditions. The use of this model should reflect the true behaviour of the process and allow distinguishing a normal mode from an abnormal one. In order to obtain this reliable model for the process dynamics, the black-box identification by means of an ARX (Auto-Regressive with eXogenous input) model based on the least squares criterion has been chosen. This study shows the choice and the performance of this modelling approach. An analysis of the inputs number, time delay and their influence on the behaviour of the prediction is carried out. A reactor-exchanger is used to illustrate the proposed ideas concerning the dynamics modelling. Satisfactory agreement between identified and experimental data is found and results show that the identified model successfully predicts the evolution of the outlet temperature of the process.

KEYWORDS: reliability; safety; modelling; ARX; reactor-exchanger

1. INTRODUCTION

Process development and continuous request for productivity led to an increasing complexity of industrial units. In chemical industries, it is absolutely necessary to control the process and any drift or anomaly must be detected as soon as possible in order to prevent risks and accidents. Moreover, detecting a fault appearance on-line is justified by the need to solve effectively the problems within a short time (Chetouani, 2006).

We are interested in the anomaly detection module intended to supervise the functioning state of the system (Chetouani, 2007). The former has to generate on-line information concerning the state of the automated system. This state is characterized not only by control and measurement variables (temperature, reaction rate, etc.), but also by the general behaviour of the process and its history, showing in time whether the behaviour of the system is normal or presents drifts. In the context of numerical control, fault detection and isolation (FDI) proves a vital complement to the adaptive means of dealing with instabilities in nonlinear highly unsteady systems. Under normal conditions, the fault detection module allows all information to be processed and managed in direct liaison with its general behaviour. In other case, it detects any anomaly and alerts the operator by setting on the appropriate alarms.

The intrinsic highly nonlinear behaviour in the industrial process, especially when a chemical reaction is used, poses a major problem for the formulation of good predictions and the design of reliable control systems (Cammarata et al., 2002). Due to the relevant number of degrees of freedom, to the nonlinear coupling of different phenomena and to the processes complexity, the mathematical modelling of the process is computationally heavy and may produce an unsatisfactory correspondence between experimental and simulated data. Similar problems arise also from the uncertainty for the parameters of the process, such as the reaction rate, activation energy, reaction enthalpy, heat transfer coefficient, and their unpredictable variations. In fact, most of the chemical and thermo-physical variables both strongly depend and influence instantaneously the temperature of the reaction mass (Chetouani, 2007). One way of addressing this problem is the use of a reliable model for the on-line prediction of the system dynamic evolution (Leontaritis et al., 1985).

The main aim of this study is to obtain a powerful model of reference allowing to reproducing the process dynamics in normal mode. The present study focuses on the development, and implementation of an ARX model for the one-step ahead forecasting of the reactor-exchanger dynamics. The performance of this stochastic model was then evaluated using the performance criteria. Results show that the ARX model is representative for the dynamic behaviour of the nonlinear process. Experiments were performed in a reactor-exchanger and experimental data were used both to define and to validate the model. The identification procedure, the experimental set-up and prediction results are described in the following sections.

2. INPUT-OUTPUT MODELLING APPROACH: ARX IDENTIFICATION

Modelling is an essential precursor in the parameter estimation process. Identification strategies of various kinds by means of input–output measurements are commonly used in many situations in which it is not necessary to achieve a deep mathematical knowledge of the system under study, but it is sufficient to predict the system evolution (Fung et al., 2003; Mu et al., 2005). This is often the case in control applications, where satisfactory predictions of the system that are to be controlled and sufficient robustness to parameter uncertainty are the only requirements. In chemical systems, parameter variations and uncertainty play a fundamental role on the system dynamics and are very difficult to be accurately modelled (Cammarata et al., 2002). Therefore, the identification approach based on input-output measurements can be applied.

In this study, the chosen method adopted for process modelling is based on a parametric identification of an ARX model. The choice of this strategy is justified by the fact that it is simple to implement it. The evolution of the estimated output allows to follow the dynamics evolution of the process and to reflect the fault presence by the variation of the estimated parameters of the identified model (Iserman, 1993).

ARX modelling was the subject of studies in several fields such as chemical engineering (Rivera et al., 1995; Rohani et al., 1999), agriculture and biological science (Fravolini et al., 2003; Frausto et al., 2003), medicine (Liu et al., 2003), energy and the power (Yoshida et al., 2001), Energy economics (Ringwood et al., 1993).

In this paper, we propose the ARX identification for modelling the dynamic behaviour of a reactor-exchanger. The aim is to analyze the model orders, the time delay and the validation of the identified model.

The ARX structure describes the input effects $u(t)$ on the process output $y(t)$. The ARX model is represented by the following expression:

$$y(t) = -a_1 y(t-1) - \cdots - a_{na} y(t-n_a) + b_1 u(t-1-n_k) + \cdots + b_{n_b} u(t-n_b-n_k) + e(t) \quad (1)$$

where $e(t)$ refers to the noise supposed to be Gaussian. a_{n_a} and b_{n_b} are the model parameters. n_a and n_b indicate respectively, the order of the polynomials of the output $A(q)$ and the input $B(q)$. The parameter n_k is the time delay between $y(t)$ and $u(t)$.

The polynomial representation of the equation (1) is given as follows:

$$A(q)y(t) = B(q)u(t-n_k) + e(t) \quad (2)$$

where $A(q)$ and $B(q)$ are given by:

$$A(q) = 1 + a_1 q^{-1} + \cdots + a_{n_a} q^{-n_a} \quad (3)$$

$$B(q) = b_1 q^{-1-n_k} + \cdots + b_{n_b} q^{-n_b-n_k} \quad (4)$$

q^{-1} is the delay operator such as:

$$u(t=1) = q^{-1} u(t) \quad (5)$$

$A(q)$ and $B(q)$ are estimated by the least squares identification (Ljung, 1987, Ljung, 2000).

3. EXPERIMENTAL RESULTS

3.1. EXPERIMENTAL DEVICE

The reactor-exchanger is a glass-jacketed reactor with a tangential input for heat transfer fluid. It is equipped with an electrical calibration heating and an input system. It is equipped with Pt100 temperature probes. The heating-cooling system, which uses a single heat transfer fluid, works within the temperature range between −15 and +200 C. Supervision software allows the fitting of the parameters and their instruction value. It displays and stores data during the experiment as well as for its further exploitation. The input of the reactor-exchanger $u(t)$ represents the heat transfer fluid temperature allowing the heating-cooling of the water. $y(t)$ represents the outlet temperature of the reactor-exchanger. The process is excited by an input signal which is very rich in frequencies and amplitudes in order to have a data set suitable for the estimation procedure. The sampling time is fixed at 2 seconds. Before starting the estimation of parameters, the database is divided into two separated sets. The first set is used for the estimation of parameters and the second one for the model validation. The first set is sufficiently informative and covering the whole spectrum. The second set contains sufficient elements to make the validation as credible as possible.

3.2. ESTABLISHMENT OF ARX MODELS

A set of models is built by fixing $n_a = [1, \ldots, 5]$, $n_b = [1, \ldots, 5]$ and $n_k = [1, \ldots, 10]$. The models having n_a lower than n_b are rejected in order to respect the physical aspect of

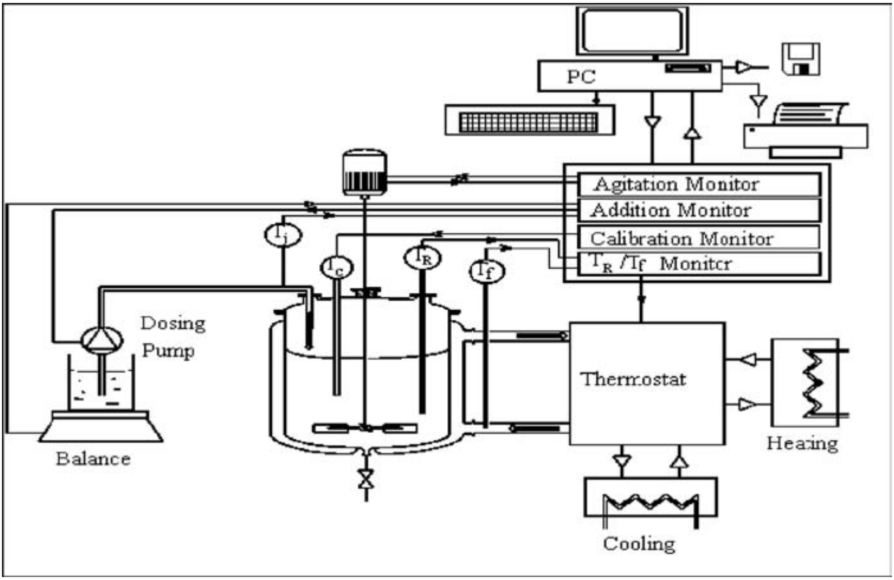

Figure 1. Experimental device: A reactor-exchanger

the process. Consequently, a set of 150 models is worked out and estimated while examining the stability of each model by the Lyapunov criterion (Ljung, 1987).

3.2.1. Estimation of the time delay

There are several methods for estimating the time delay (Ljung, 1987; Chen et al., 1989; Ljung, 2000). In this paper, the adopted approach is based on the evaluation of the quadratic criterion (Ljung, 2000). This criterion is as follows:

$$V(\theta) = \frac{1}{N}\sum_{t=1}^{N}\varepsilon(t,\theta)^2 \tag{6}$$

$\varepsilon(t,\theta) = y(t) - \hat{y}(t)$ and $\hat{y}(t)$ represent respectively the prediction error and the associated predictor. The quadratic criterion value is calculated in function of the time delay value $n_k = [1, \ldots, 10]$. This method is applied to two simple ARX models ($n_a = n_b = 1$) and ($n_a = n_b = 2$). The choice of these simple models allows observing the criterion evolution according to the time delay but without compensating it (time delay) by a high complexity model. The criterion evolution according to the time delay for those simple models is shown in figs. 2 and 3.

By examining fig. 3, it is easy to observe the presence of the minimal value of the criterion for $n_k = [5,6,7,8]$. But, in fig. 2, this presence is supported clearly for $n_k = [6,7]$.

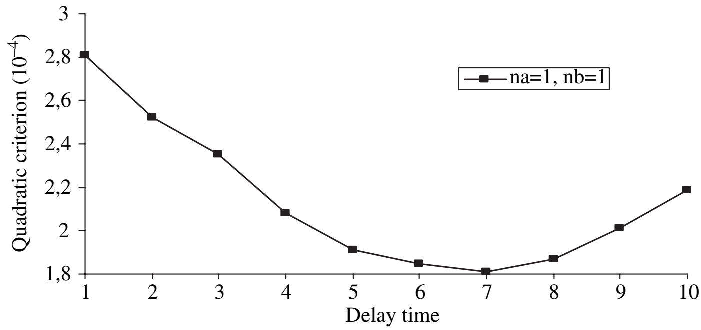

Figure 2. Criterion evolution according to the time delay n_k for $n_a = n_b = 1$

Therefore, it is better to consider, first, that the time delay values are both $n_k = 6$ and $n_k = 7$. Then, each model having a different time delay ($n_k = [6,7]$) will be rejected.

3.2.2. Quality of fit

The quality of fit criterion allows a judicious selection of models. This criterion proposed by Hagenblad et al. (1998) is based on the analysis of the prediction error and of the output variance. It is given by the following expression:

$$Q = 100 \times \left(1 - \sqrt{\sum_{k=1}^{N} \left(\hat{y}(k) - y(k) \right)^2} \Bigg/ \sqrt{\sum_{k=1}^{N} \left(y(k) - \frac{1}{n} \sum_{i=1}^{n} y(i) \right)^2} \right) \tag{7}$$

Fig. 4 shows the criterion evolution according to the different models $M_{n_a \,.\, n_b}$. The models $M3.2$, $M4.2$ and $M5.5$ have a good quality of adjustment compared to the other models

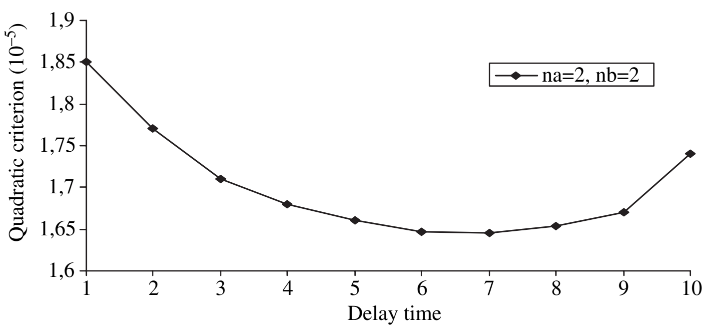

Figure 3. Criterion evolution according to the time delay n_k for $n_a = n_b = 2$

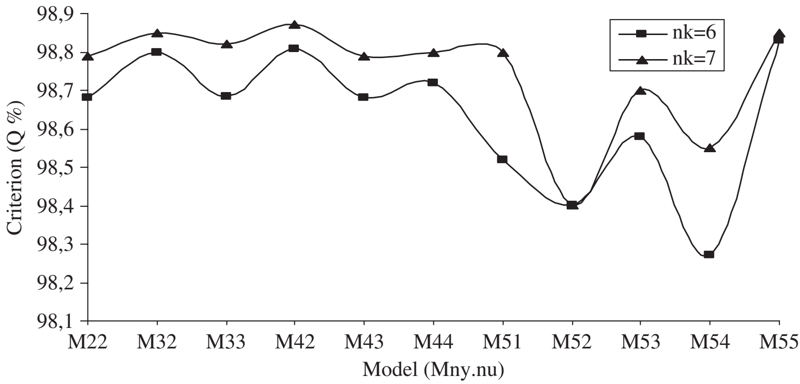

Figure 4. Criterion evolution according to the different models $M_{n_a \cdot n_b}$

(important peaks). The model $M5.5$ is not being chosen because it is too large. The peak of the model $M4.2$ is more important than that of the model $M3.2$. Consequently, the model $M4.2$ is more representative for the dynamic behaviour than the model $M3.2$ and thus for the two time delay values ($n_k = 6$ and $n_k = 7$). In conclusion, the model ($M4.2.7$) having $n_k = 7$ is the most suitable one for reproducing the process dynamics.

3.3. RESIDUAL ANALYSIS

Once the training and the test of the ARX model has been completed, it should be ready to simulate the system dynamics. Model validation tests should be performed to validate the identified model. Billings et al. (1986) proposed some correlations based model validity tests. In order to validate the identified model, it is necessary to evaluate the properties of the errors that affect the prediction of the outputs of the model, which can be defined as the differences between experimental and simulated time series. In general, the characteristics of the error are considered satisfactory when the error behaves as white noise, i.e. it has a zero mean and is not correlated (Cammarata et al., 2002; Billings et al., 1986). In fact, if both these conditions are satisfied, it means that the identified model has captured the deterministic part of the system dynamics, which is therefore accurately modelled. To this aim, it is necessary to verify that the auto-correlation function of the normalized error $\varepsilon(t)$, namely $\phi\varepsilon\varepsilon(\tau)$, assumes the values 1 for $t = 0$ and 0 elsewhere; in other words, it is required that the function behaves as an impulse. This auto-correlation is defined as follows (Zhang et al., 1996; Billings et al., 1986):

$$\phi\varepsilon\varepsilon(\tau) = E(\varepsilon(t-\tau)\varepsilon(t)] = \delta(\tau) \qquad \forall\tau, \tag{8}$$

where ε is the model residual. $E(X)$ is the expected value of X, τ is the lag.

This condition is, of course, ideal and in practice it is sufficient to verify that $\phi\varepsilon\varepsilon(\tau)$, remains in a confidence band usually fixed at the 95%, which means that $\phi\varepsilon\varepsilon(\tau)$ must remain inside the range $\pm\frac{1.96}{\sqrt{N}}$, with N the number of testing data on which $\phi\varepsilon\varepsilon(\tau)$ is calculated.

Billings et al. (1986) proposed also tests for looking into the cross-correlation among model residuals and inputs. This cross-correlation is defined by the following equation:

$$\phi u\varepsilon(\tau) = E(u(t-\tau)\varepsilon(t)) = 0 \qquad \forall\tau \tag{9}$$

To implement these tests (8, 9), u and ε are normalized to give zero mean sequences of unit variance. The sampled cross-validation function between two such data sequences *u(t)* and $\varepsilon(t)$ is then calculated as:

$$\phi u\varepsilon(\tau) = \frac{\sum_{t=1}^{N-\tau} u(t)\varepsilon(t+\tau)}{\left(\sum_{t=1}^{N} u^2(t)\sum_{t=1}^{N}\varepsilon^2(t)\right)^{1/2}} \tag{10}$$

If the equations (8, 9) are satisfied then the model residuals are a random sequence and are not predictable from inputs and, hence, the model will be considered as adequate. These correlations based tests are used here to validate the neural network model. The results are presented in fig. 5.

In these plots, the dash dot lines are the 95% confidence bands. Fig. 5 shows that the evolution of the cross-correlation of the ARX model is inside the 95% confidence bands. The auto-correlation of the ARX model exceeds the threshold (95%) for few points. This explains the non-dependence of the residual signal from the input one. Therefore, this model is considered a reliable one for describing the dynamic behaviour of the process. Fig. 6 represents the prediction error between the real output temperature and the estimated one.

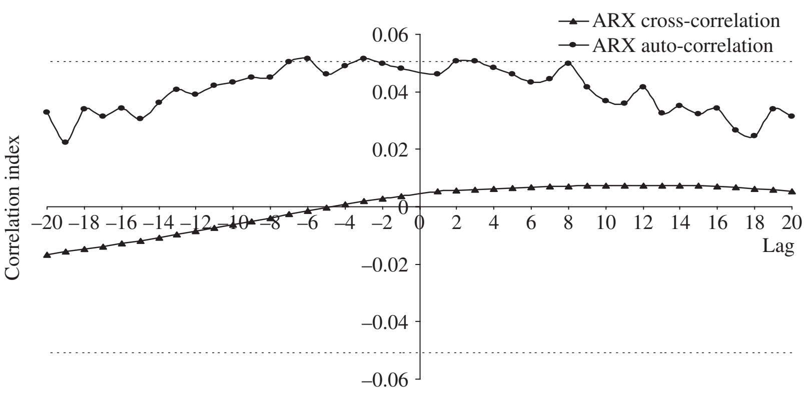

Figure 5. Results of model validation tests

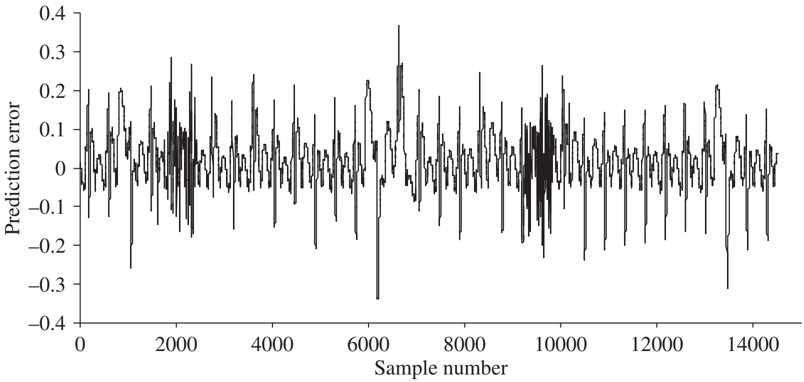

Figure 6. Prediction error of the output temperature

The main advantage of the proposed approach consists in the natural ability of the ARX approach in modelling nonlinear dynamics in a fast and simple way and in the possibility to address the process to be modelled as an input-output black-box, with little or no mathematical information on the system.

4. CONCLUSION

This work aims to identify process dynamics by means of an ARX model in order to provide reliable predictions. This study shows that the identification of the reactor-exchanger dynamics by means of input-output experimental measurements provides a useful solution for the formulation of a reliable model. In this case, the results showed that the model is able to give satisfactory descriptions of the experimental data. Finally, the identified model will be useful as a reference one for the fault detection and the isolation (FDI) which can occur through the process dynamics.

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