IMPROVED ADAPTIVE DYNAMIC CONTROL OF A POLYMERIZATION PROCESS

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ABSTRACT

In this paper an appropriate paradigm of multi-variable dynamic systems of strong non-linear coupling, a polymerization process is considered. Since the state propagation of the various internal degrees of freedom cannot directly be controlled, and the desired output is nonlinear function of these quantities, adaptive control is needed even in the possession of the exact dynamic model. Only a single input variable is used as the control signal and a single output variable is observed. Considering the details of the dynamics of the transitions between different steady states the role of choosing proper sampling rate is analyzed. The conclusions are justified by simulation results.

KEYWORDS: Adaptive Control, Polymerization Process, Chemical Reactions.

1. INTRODUCTION

An important class of physical systems' control is the set of dynamic processes in which some deterministic response to an external input is expected. This is typically relevant, for instance, in the realm of chemical processes that correspond to the state propagation of multivariable systems in which only certain degrees of freedom are directly observed and controlled, while the other ones behave according to the internal dynamics of the systems. In such cases, being in lack of knowledge on the exact state of the system to be controlled, even in the possession of the exact dynamic system model some adaptive technique is necessary to obtain acceptable control quality. In general it evidently does not seem to be likely to successfully establish this adaptation on the identification of the parameters of an analytically formulated "white box model". Instead of that simpler techniques as e.g. soft computing approaches may be used. For instance, discrete time model can be formulated in the form of a difference equations with an external input that usually is known quantity (*Autoregressive Moving Average Model with eXternal input - ARMAX*) [1]. This approach serves as a paradigm for various particular approaches. E.g. in the so-called Takagi-Sugeno fuzzy models the consequent parts are expressed by analytical expressions similar to that of the ARMAX form. Alternative possibilities are provided by Neural Networks that in general are useful means of developing nonlinear models, e.g. in the linearization of the nonlinear characteristics of various sensors [2]. Neuro-fuzzy systems automatically tune the fuzzy system by using *Neural Networks* (*NNs*). The *Adaptive Neuro-Fuzzy Inference System* (*ANFIS*) is a combination of an artificial neural network and a *Fuzzy Inference System* (*FIS*) [3]. *Radial Basis Function Networks* (*RBFNs*) are attractive alternatives to the standard *Feedforward Networks* using backpropagation learning technique [4]. In fact the nodes of a RBFN represent "fuzzified" or "blurred" regions which correspond to the well defined antecedent sets of a fuzzy controller. In many cases development of the whole model is a complicated task especially when the "antecedent" part is strongly nonlinear multivariable function of the input. Evolutionary methods as e.g. the *Particle Swarm Optimization* that realizes stochastic random search in a multi-dimensional optimization space [5] may be combined with them. In the case of certain problem classes similarity relations can also be observed and utilized to simplify the design process [6].

A significant common feature of the above approaches is that they try to develop a "complete" soft computing based model of the system to be controlled. This naturally makes the question arise whether it is always reasonable to try to identify a "complete" model. As a plausible alternative simple adaptive controllers can be imagined that do not wish to create "complete" and "everlasting" models. Instead of that on the basis of slowly fading recent information a more or less temporal model can be constructed and updated step by step by the use of simple updating rules consisting of finite algebraic steps of lucid geometric interpretation. At the Budapest Tech two variants of this simple approach were elaborated and extensively investigated. One of them is based on the modification of the renormalization transformation extensively used in various fields of physics (e.g. [7]), the other one is based on a lucid geometric interpretation of the ARMAX-type approaches using floating system of basis vectors for describing the controlled system [8]. Though the convergence of the method in [7] can be guaranteed for a quite wide class of physical systems (e.g. for Classical Mechanical Systems), the latter one in [8] does not need so rigorous conditions.

This latter method was already applied for the control of the presently addressed 2nd order polymerization process in a 1st order approach in the "quasi-stationary" limit, i.e. when the chemical process is considered as a consecutive set of states of thermal equilibrium [9]. The 1st order approach was possible due to using a relatively big cycle time during which the most essential parts of stationary state to stationary state transitions generated by the abrupt jumps of the control signal already took place, and their averages during the sampling (cycle) time resulted in more or less useful measures. However, this approach had very much limited accuracy and it was concluded that for its improvement taking into consideration the 2nd order dynamics is needed as well as choosing proper sampling time during which the significant dynamic effects cannot be averaged out. The first step in this direction was made in [10] by using a very primitive adaptation rule. Though the quality of the control was considerably improved with respect to that of [9], the available accuracy still considerably depended on the sampling time even within the region that should have been fine enough for revealing essential dynamic details of the process. In the sequel this method will be further improved. Furthermore, it will be proved that though formally the behavior of this chemical process has strong and essential similarity with that of the Classical Mechanical Systems, the control approach of [7] cannot directly applied to it. A brief explanation of this fact consists in observing that though this chemical process has the "counterpart" of the inertia parameters of the Classical Mechanical Systems, these "chemical inertias" vary very rapidly during the relaxation process between two adjacent steady states, in contrast to the mechanical "inertias" that remain approximately constant during a small variation of the configuration. In the sequel at first the mathematical model and detailed analysis of the polymerization process is presented. Following that the improved control approach is detailed, finally simulation results and concluding remarks are given.

2. THE MODEL OF THE POLYMERIZATION PROCESS

The chemical reaction considered is the free-radical polymerization of methyl-metachrylate with azobis(isobutyro-nitrile) as an initiator and toluene as a solvent taking place in a jacketed *Continuous Stirred Tank Reactor* (*CSTR*). The mathematical model of this process was taken from [11]. In his Doctoral Thesis J. Madár applied a sophisticated approach based on *Genetic Programming* (*GP*) for identifying this reaction [12]. The aim of the present paper is to investigate a more simple temporal identification approach for this system. According to [11] the model considered takes into account the conservation of the atoms in the chemical processes, and contains the state variables x_1, …, x_4 denoting *dimensionless* concentrations of various chemical components taking part in the reaction. For our purposes the really interesting variables are x_1 i.e. the monomer concentration, and the output of the system, that is the *number-average molecular weight* denoted by y.

$$\dot{x}_1 = A(B - x_1) - Cx_1x_2^{1/2}, \quad \dot{x}_2 = Du - Ex_2$$
$$\dot{x}_3 = FCx_1x_2^{1/2} + Gx_2 - Hx_3, \quad \dot{x}_4 = Ix_1x_2^{1/2} - Jx_4, \quad y := \frac{x_4}{x_3} \tag{1}$$

The *process input*, that is the control signal, u is the *dimensionless volumetric flow rate of the initiator*. The constants in Eq. (1) have the following numerical values: A=10, B=6, C=2.4568, D=80, E=10.1022, F=0.024121, G=0.112191, H=10, I=245.978, and J=10. It was shown via perturbation calculus in [9] that for a constant process input u Eq. (1) yields *stable stationary solutions* in which the time-derivatives of the state variables are equal to zero. It was also concluded that at the time-scale commonly used in industrial control of such reactions (about 0.1-0.2 s sampling time) the internal dynamics of the system achieves its stable stationary states between two control actions with a rough approximation. Consequently, in the applied ARMAX-type control instead of the *internal dynamics* of the system rather the "dynamics" of the desired output was revealed. In order to achieve a more accurate control it is expedient to take it into account that we have special functions as $y(x)$, $\dot{y}(x,\dot{x})$, therefore $\dot{y}(u,x)$, and $\ddot{y}(u,\dot{u},x)$. More specifically, according to Eq. (1)

$$\dot{y} = \dot{x}_4x_3^{-1} - x_4x_3^{-2}\dot{x}_3, \quad \ddot{y} = \ddot{x}_4x_3^{-1} - 2\dot{x}_4x_3^{-2}\dot{x}_3 - 2x_4x_3^{-3}\dot{x}_3^2 - x_4x_3^{-2}\ddot{x}_3 \tag{2}$$

For the 2nd time-derivatives from Eq. (1) it is obtained that

$$\ddot{x}_4 = I\dot{x}_1x_2^{1/2} + 0.5Ix_1x_2^{-1/2}\dot{x}_2 - A\dot{x}_4, \quad \ddot{x}_3 = F\dot{x}_1x_2^{1/2} + 0.5Fx_1x_2^{-1/2}\dot{x}_2 + D\dot{x}_2 - H\dot{x}_3 \tag{3}$$

Since in the whole $\{\dot{x}_i\}$ set only $\dot{x}_2$ depends directly on u, it is obtained that

$$\ddot{y}(u,x) = \tilde{a}(x)u + \tilde{b}(x) \equiv [\partial\ddot{y}/\partial u](x)u + \tilde{b}(x). \tag{4}$$

Eq. (4) evidently is very similar to the motion of a mass point of non-constant "inertia" $\tilde{a}^{-1}$ under a "control" and an external "force" together $(u + \tilde{b}/\tilde{a})$. In Figure 1 calculations are given for a drastic jump of u from 0.005 to 0.015. It is evident that the transient is "completed" during approximately 0.67 s, but during this short process both the "inertia" as well as the "disturbance force" suffers quite significant and fast variation. Furthermore, the "inertia" in this process is *negative*. The negative inertia itself would not mean serious difficulty in applying the method given in [7], but the very fast variation of the "inertia" and the "external force" can make its convergence dubious. On this reason in the sequel an adaptive controller based on a philosophy similar to that of the fuzzy controller will be developed and investigated.

3. THE PROPOSED CONTROL AND SIMULATION RESULTS

For control purposes exponential tracking error relaxation can be prescribed on a purely "kinematic" basis determining the "*desired acceleration*" $\ddot{y}^D$ as

$$\ddot{y}^D = \ddot{y}^N + \tilde{D}(\dot{y}^N - \dot{y}) + \tilde{P}(y^N - y). \tag{5}$$

in which the indices "D" and "N" refer to the "*desired*" and the "*nominal*" values, respectively, $\tilde{D} \approx 2/T_{\exp}$, and $\tilde{P} = 0.5\sqrt{0.8}\tilde{D}$. This choice corresponds to two slightly different time-constants of error relaxation without oscillation about T_{exp}. In order to realize Eq. (5) an intentionally roughly estimated value is used for $\tilde{a}$ as K=-3×10^7, and in the non-adaptive control the following estimation is used for updating the control signal:

$$u(t+\delta t) = u(t) + \left[\ddot{y}^D(t) - \ddot{y}(t-\delta t)\right]/K \tag{6}$$

In Eq. (6) K serves as a "*rough system model*". To improve the control defined in Eq. (6) the following *modified updating rules* were applied for u using a multiplication factor $s(t)$:

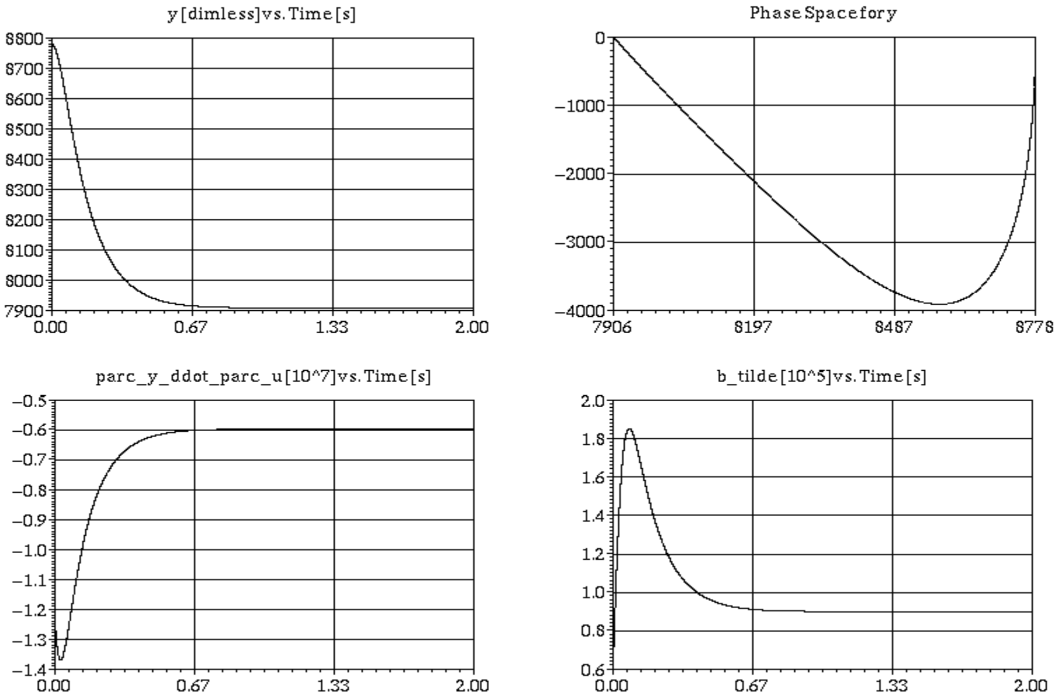

Figure 1. Relaxation of the stationary state for a "drastic" jump by the control signal u from *0.005 to 0.015:* $y(t)$ and $\dot{y}$ vs. y (1st raw), $\tilde{a}(t)$ and $\tilde{b}(t)$ (2nd raw).

$$
\begin{aligned}
&u(t+\delta t)=u(t)+s(t)\left[\ddot{y}^D(t)-\ddot{y}(t-\delta t)\right]/K\\
&if\ \ddot{y}^D>0\ then\ if\left(\ddot{y}^D>\ddot{y}\ then\ s(t+\delta t)=\zeta s(t)\ else\ s(t+\delta t)=s(t)/\zeta\right)\\
&if\ \ddot{y}^D<0\ then\ if\left(\ddot{y}^D<\ddot{y}\ then\ s(t+\delta t)=\zeta s(t)\ else\ s(t+\delta t)=s(t)/\zeta\right)
\end{aligned}
\tag{7}
$$

in which the $1<\zeta<<2$ term also depends on the time as

$$
\zeta=1+\min\left(\eta_{\max},\eta_{\min}+[\eta_{\max}-\eta_{\min}]\times\left|\ddot{y}^D-\ddot{y}\right|/\Delta\right),
\tag{8}
$$

in which $0<\eta_{min}<\eta_{max}<<1$, and Δ approximates the maximum of the observable "*acceleration error*". In Eq. (7) the cycle time δt and a constant ζ together determine *a rigid (fixed) adaptation speed* that, according to [10], was not flexible enough. This situation is improved by Eq. (8) expressing the simple rule that the greater the acceleration error the higher speed of adaptation is needed (of course, only within certain limits determined by the *max* function).

Figure 2 well reveals the insufficient nature of the non-adaptive control by describing the phase trajectories of the nominal (egg-shaped "canonical" curves) and the simulated (non-canonical curves) motions. It is interesting that the richer the dynamics of the motion (i.e. the shorter the cycle time used for averaging the observation) the lower the quality of the non-adaptive control is. On the basis of calculations made for the non-adaptive control the following parameters were roughly estimated/proposed for the *adaptive* control: $\eta_{min}=10^{-3}$, $\eta_{max}=1.5\times10^{-2}$ *dimensionless,* $\Delta=10^4\ s^{-2}$. In Figure 3 the operation of the adaptive counterpart of the worst result in Figure 2 is described. Even the comparison only of the phase trajectories convinces the reader on the superiority of the adaptive approach. The "fuzzy" shape of the curve of tracking error suggests that the dynamic details revealed in Figure 1 are now taken into consideration by the adaptive controller. The considerable modification of the adaptive factor with respect to 1 and its fast dynamic variation in time testifies that the considerable improvement is the result or consequence of the adaptation process.

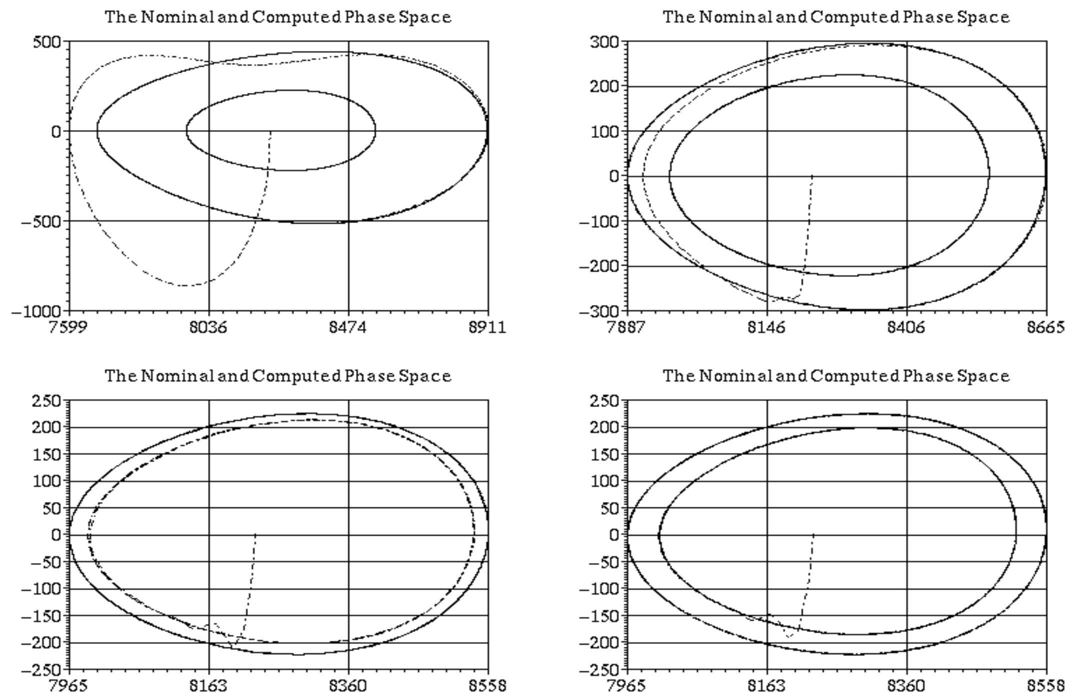

Figure 2. The phase trajectory tracking of the non-adaptive control according to Eq. (6) for increasing cycle time: δt=0.067/4 s (upper left), δt=0.067/2 s (upper right), δt=0.067 s (lower left), and δt=0.08 s (lower right).

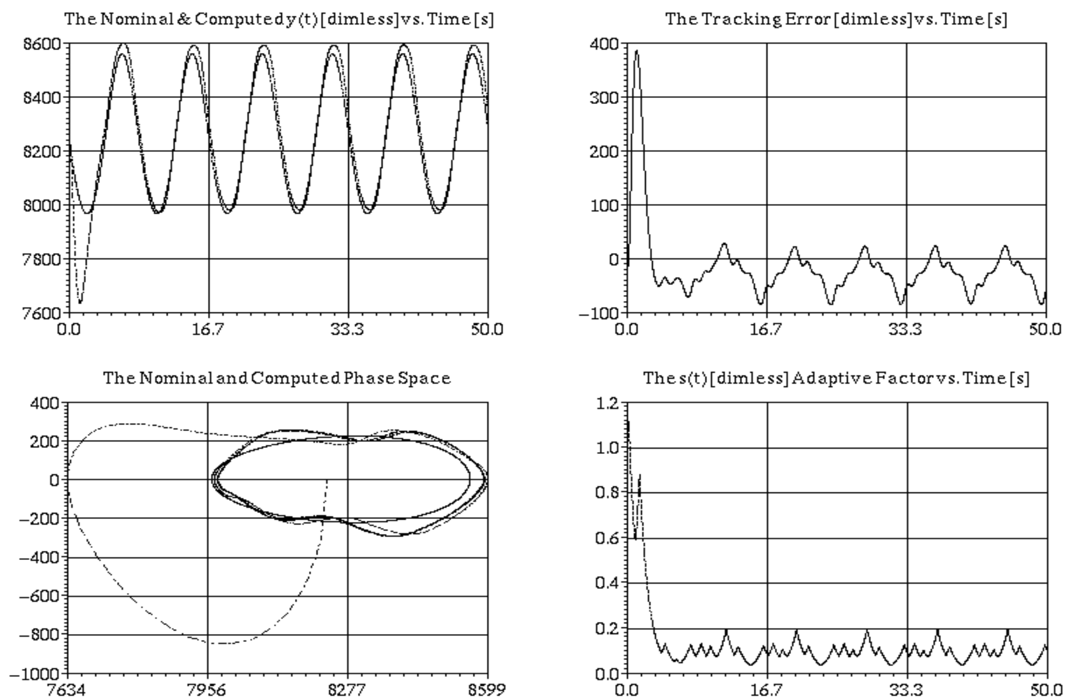

Figure 3. The operation of the adaptive control for cycle time: δt=0.067/4 s: trajectory tracking (upper left), trajectory tracking error (upper right), the phase trajectory tracking (lower left), and the adaptive factor s(t) (lower right).

4. CONCLUSIONS

Detailed dynamic analysis of a particular polymerization process revealed that if considerable modification in the process output is needed during the time-interval of 8-18 *s*, approximately a $\delta t = 0.067/4\ s$ cycle time is needed, that means much more frequent sampling than the usual 0.2 *s* applicable for far slower industrial processes. For this purpose a special, improved adaptive controller was constructed and investigated via simulation.

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