Sophisticated Dynamic Adaptive Control of a Polymerization Process

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Abstract: The chemical process considered serves as an appropriate paradigm of multivariable dynamic systems of strong non-linear coupling in the control of which the state propagation of various internal degrees of freedom can neither be measured nor directly controlled. The desired output is a single real, nonlinear function of these quantities. In the present example only a single input variable is used for control purposes. In the paper quantitative model of the process is presented. For controlling this process various approaches were applied: genetic programming for the identification of the process, an ARMAX-type floating basis vector approach in the quasi-stationary limit, and fuzzy-type adaptive control with fixed and with variable speed in which the adaptation rule was determined on qualitative considerations. In the present approach the adaptation rule is determined in a sophisticated manner, on the basis of a modified version of the renormalization transformation, in which the system is observed real time. The quality of the control is investigated via simulation from the points of view of its robustness with respect to setting its free parameters, and sensitivity to the measurement noises. It is concluded that at the time-scale of about 0.067 s sampling time the 'dynamics' of the controlled process can well be traced, and on the basis of a simple planning method quite accurate dynamic control can be achieved.

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 a multivariable system in which only certain degrees of freedom are directly observed and controlled, while the other ones behave according to the internal dynamics of the system.

In general for such systems discrete time models can be formulated in the form of difference equations with an external input that usually is known quantity

(Autoregressive Moving Average Model with eXternal input - ARMAX) [1]. In more sophisticated models as in the so-called Takagi-Sugeno fuzzy models the consequent parts are expressed by analytical expressions similar to that of an ARMAX model, and they use some linear combinations of such rules in which the coefficients depend on the antecedents. With the help of such Takagi-Sugeno fuzzy IF-THEN rules sufficient conditions to check the stability of fuzzy control systems are now available e.g. [2]. As alternative control approaches Neural Networks can be mentioned that in general are useful means of developing nonlinear models. A particular case of such applications is when the model itself consists of certain nonlinear mapping, for instance in the linearization of the nonlinear characteristics of various sensors [3]. Neuro-fuzzy systems provide the fuzzy systems with the possibility of automatic tuning by using Neural Network (NN) as a tool. The Adaptive Neuro-Fuzzy Inference System (ANFIS) is a cross between an artificial neural network and a Fuzzy Inference System (FIS) [2, 4, 5, 6]. The adaptive network can be a multi-layer feed-forward network in which each node (neuron) performs a particular function on incoming signals. Radial Basis Function Networks (RBFNs) provide an attractive alternative to the standard Feedforward Networks using backpropagation learning technique [7]. The linear weights associated with the output layer can be treated separately from the hidden layer's neurons. 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 [8, 9] 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 [10].

A significant common feature of the above approaches is that they try to develop a 'complete' and 'permanent' 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' and 'permanent' model especially in practical situations in which no full information is available for the process via real-time observation. As a plausible alternative simple adaptive controllers can be imagined that do not wish to create a 'complete, permanent' model. Instead of that a more or less temporal model can be constructed that establishes/identifies a mapping between the known excitation and the observed response of the controlled system. This model cannot be 'complete', because this relationship may depend on the exact physical state of the system the unobserved variables of which also vary in time. Furthermore, the observed response may belong to the combination of the 'known' and the 'unknown' parts of the physical actions exciting the system. On this reason the mapping cannot be permanent, and needs continuous updating. In the past few years at the Budapest Tech two variants of this simple approach were elaborated and extensively investigated via simulation results. One of them is based on a lucid geometric interpretation of the ARMAX-type approaches using floating system of basis vectors for describing the controlled system [11], the other one uses a modification of the renormalization transformation extensively used in various fields of physics (e.g. [12]). Though the convergence of the method in [12] can be guaranteed for a quite wide class of physical systems (e.g. for Classical Mechanical Systems), for this particular chemical reaction it cannot be applied. This method later was extended to an even wider class of physical systems in [13], in which a particular case, the control of an indirectly driven axis of a mechanical system was considered as an application paradigm. A comparative analysis of the operation of these different methods was given in connection with the control of a Classical Mechanical System in [14].

In the present paper the more sophisticated, extended method is applied for the control of a chemical process, namely to 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 (JCSTR). The mathematical model of this process was taken from [15]. In his Doctoral Thesis J. Madár applied a sophisticated approach based on Genetic Programming (GP) for identifying this reaction [16]. The method of [11] was already successfully applied for the control of this process in its quasi-stationary limit in [17]. On the basis of a detailed dynamic analysis it was observed that for efficient adaptive control of this system introduction of *a single adaptive parameter is satisfactory* for the tuning of which *simple rules can be established*. In this manner a dynamic control applied in a finer time scale than that of [11] became available with *fixed tuning rate* in [18], and in a more developed version with *varying tuning rate* in [19]. On the basis of these solutions formally perfect fuzzy controllers could be developed that operates on the basis of the following principle: *the greater the control error is the higher speed of adaptation is needed*.

Instead of applying some fuzzy rules, the approach in the present paper tries to *exactly establish the parameter tuning* on the basis of the observation that the conditions needed for the convergence of the extended modification of the renormalization transformation are valid in the case of this chemical reaction. In the sequel the control method is described in general then the quality of the control is investigated via simulation from the points of view of its robustness with respect to setting its free parameters, and sensitivity to the measurement noises.

2 The Proposed Control Approach

The forthcoming considerations pertain to physical systems for which the controller tries to obtain a *desired response* x^d by applying an imprecise and incomplete model to calculate the estimated necessary excitation $e=\varphi(x^d)$ that according to the actual dynamics of the system results in the realized response $x^r=\psi(\varphi(x^d))\equiv f(x^d)$. It is supposed that the desired response is known, the realized response is measurable, and though the exact form of $f(x^d)$ is not known at least its increasing or decreasing nature can be deduced from the physics of the system to be controlled. In the ideal situation the realized response is equal to the desired one that corresponds to finding the fixed point of f as $f(x^d)=x^d$.

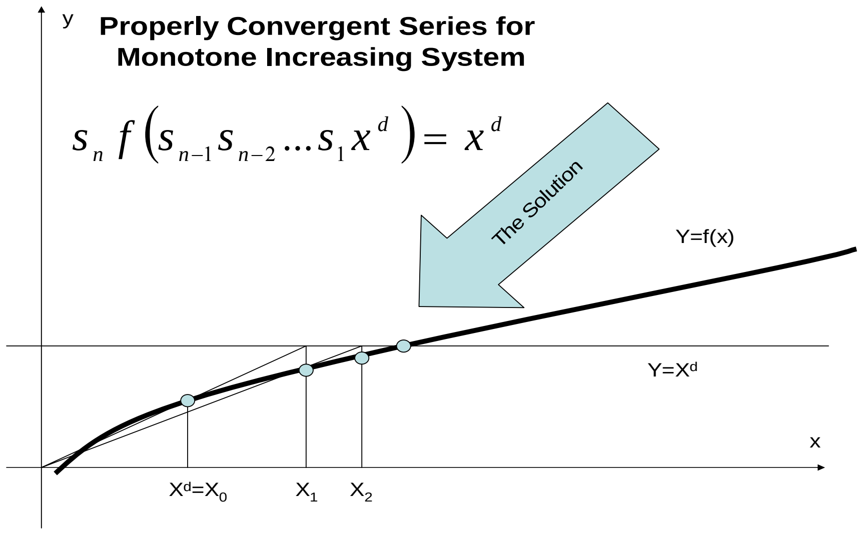

Figure 1
Possible convergence of the *Modified Renormaliaztion Transformation* based algorithm

As is well known the *Renormalization Transformation* can transform a function $f(x)$ by a scalar parameter γ as $f_\gamma(x)\equiv\gamma^{-1}f(\gamma x)$ that transforms the fixed point $f(x)=x$ since if $z=f_\gamma(z)\equiv\gamma^{-1}f(\gamma z)$ then $f(\gamma z)=\gamma z=x$. It was plausible to try to use this transformation for the adaptive control that can also be formulated as a fixed point problem. However, due to the fact that in the control just x^d is needed as the output, the *modified algorithm* defined as

$$s_n f\left(s_{n-1}s_{n-2}...s_1x^d\right)=x^d \tag{1}$$

was introduced in [20]. As it qualitatively is illustrated in Fig. 1 for monotone increasing system this series can be properly convergent ($s_n\to1$) depending on how the solution of the $f(sx^d)=x^d$ equation is situated in the system of coordinates of the appropriate figure. (Divergent solutions can also be constructed). *For monotone decreasing SISO systems* it was a plausible idea to extend the above given transformation by a parameter ζ that can either be positive or negative, and that for the special case of $\zeta=0$ corresponds to the original transformation [Fig. 2].

$$s_n f\left(x_{n-1}\right)=f\left(x_{n-1}\right)+\zeta\left(f\left(x_{n-1}\right)-x^d\right),\ x_n=s_nx_{n-1},\zeta>0 \tag{2}$$

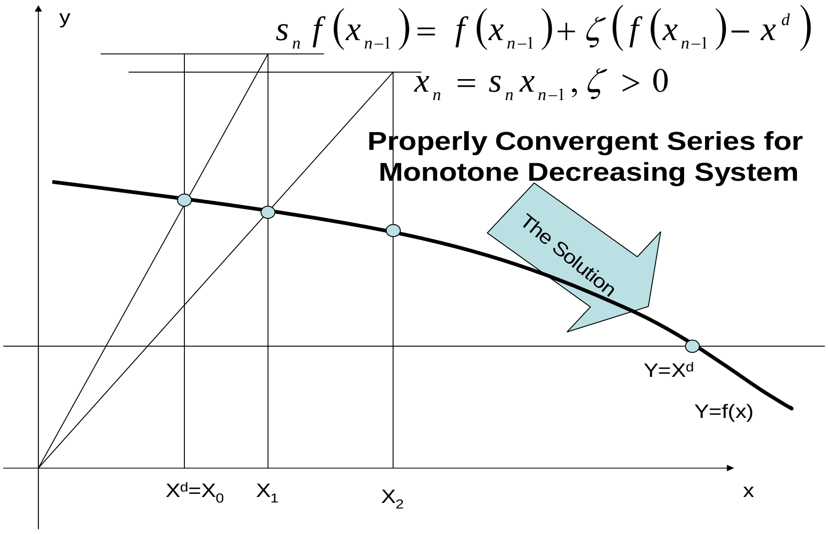

Figure 2
Proper convergence of the Extended Modified Renormaliaztion Transformation

To give a satisfactory condition for the convergence of the proposed method consider *a flat differentiable function* $g(x)$, for which the following estimations can be done according to which if the derivative of g is small enough in a region it realizes a contractive mapping.

$$|g'(x)| \le K < 1,\; g(b) - g(a) = \int_a^b g'(t)dt,\; |g(b) - g(a)| \le \int_a^b |g'(t)|dt \le K|b-a| \tag{3}$$

For a *contractive mapping* the $x_n = g(x_{n-1})$ series is a Cauchy series since

$$\begin{aligned} |x_{n+1} - x_n| &= |g(x_n) - g(x_{n-1})| \le K|x_n - x_{n-1}| = K|g(x_{n-1}) - g(x_{n-2})| \le \ldots \le \\ &\le K^n |x_1 - x_0| \xrightarrow[n\to\infty]{} 0 \end{aligned}. \tag{4}$$

In a *complete metric space* that converges to a well defined value u that must be the fixed point $u = g(u)$ since

$$\begin{aligned} |g(u) - u| &\le |g(u) - x_n + x_n - u| \le |g(u) - x_n| + |x_n - u| = |g(u) - g(x_{n-1})| + |x_n - u| \le \\ &\le K|u - x_{n-1}| + |x_n - u| \xrightarrow[n\to\infty]{} 0 \end{aligned} \tag{5}$$

The series defined in (2) corresponds to seeking the solution of the following fixed point problem in which $g_\zeta(x)$ has to be contractive:

$$x_n = \frac{f(x_{n-1}) + \zeta\left(f(x_{n-1}) - x^d\right)}{f(x_{n-1})} x_{n-1} \Rightarrow x = g_\zeta(x) := \frac{f(x) + \zeta\left(f(x) - x^d\right)}{f(x)} x \quad (6)$$

In the above expression parameter ζ corresponds to the 'multiplicative' factor. In order to obtain more 'treatable' behavior when the fixed point is zero, it is expedient to introduce a 'shift' parameter D in the formula determining the multiplication factor. If $f(x)\to 0$ then $f(x)+D\to D$ and the division in (6) will not become critical:

$$x = g_{\zeta,D}(x) := \frac{f(x) + D + \zeta\left(f(x) + D - \left[x^d + D\right]\right)}{f(x) + D} x \quad (7)$$

As it is intuitively shown in Fig. 2, in many cases this extended iteration can be convergent. In the sequel it will be shown that in the case of the polymerization process just the situation qualitatively described in Fig. 2 prevails. Therefore proper designing of the control consists in roughly determining some values for the two parameter ζ and D. *Robustness of the control with respect of these parameters means that no exact setting is needed for them. Their actual setting concerns the quality of the tracking of the control but does not influence the fact of the convergence.*

3 The Model of the Polymerization Process

According to [15] the model of the polymerization process is given by the set of equations as:

$$\begin{aligned} &\dot{x}_1 = A(B - x_1) - Cx_1 x_2^{1/2}, \quad \dot{x}_2 = Du - Ex_2 \\ &\dot{x}_3 = FCx_1 x_2^{1/2} + Gx_2 - Hx_3, \quad \dot{x}_4 = Ix_1 x_2^{1/2} - Jx_4 \\ &y := \frac{x_4}{x_3} \end{aligned} \quad (8)$$

in which the state variables $0<x_1, \ldots, x_4$ denote *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. The *process input*, that is the control signal, $0<u$ is the *dimensionless volumetric flow rate of the initiator*. It is worth noting that though certain negative values for u may have physical meaning (i.e. a kind of subtraction of the initiator from the system), its practically realizable values are only non-negative numbers. The constants in (8) 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 easily shown that for a constant process input u (8) yields a *stationary solution* in

which the time-derivatives of the state variables are equal to zero [17]. In the same paper it was also shown via perturbation calculation that these stationary solutions are stable with respect to small perturbations. Detailed analysis in [19] revealed that the second time-derivative of the process output *y* depends on the system's state and the process input in a very special form as

$$\ddot{y}(\mathbf{x},u)=\tilde{a}(\mathbf{x})u+\tilde{b}(\mathbf{x}) \tag{9}$$

That is very similar to the behaviour of the Classical Mechanical Systems with the exception that the system's inertia $a(\mathbf{x})$ is not constant but strongly varies with the state **x**. However, particular model calculations showed that even for abrupt jumps in *u* this inertia $\tilde{a}$ remains negative number, and the additional term $\tilde{b}$ that is similar to a presence of some external force is positive. Therefore if the *excitation of the system* is identified with the process control input *u*, the response corresponds to d^2y/dt^2, and just the situation outlined in Fig. 2 occurs in the control. Fig. 3 revelas illustrative details of the behavior of $y(t)$ for a drastic jump of *u* from 6×10^{-3} to 1.5×10^{-2}. The simulation results presented in the sequel belong to a controller rougly designed on the numerical resulst presented in Fig. 3.

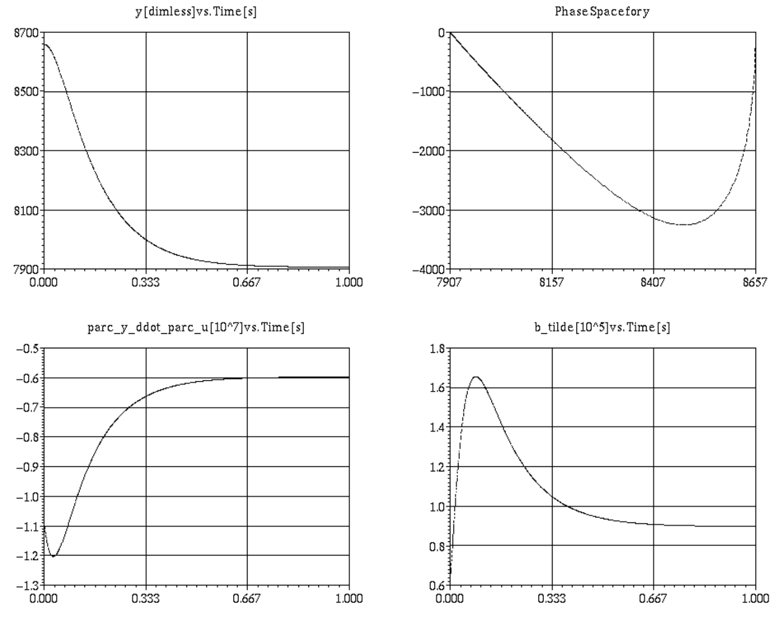

Figure 3

The reaction of the system starting from an initally stationary state belonging to $u=6\times10^{-3}$ for its abrupt jump to $u=1.5\times10^{-2}$: the variation of $y(t)$ and its phase space (1^{st} row), and that of $\tilde{a}$ and $\tilde{b}$.

4 Simulation Results

In the forthcoming simulation examples δt=0.067 *s* sampling (cycle) time was supposed for the controller, while the numerical calculation of the transients within the system was calculated with δt_{int}=1 *ms* step length. For the process output the following 'kinematic trajectory tracking' was prescribed:

$$\ddot{y}^D = \ddot{y}^N + \tilde{D}\left(\dot{y}^N - \dot{y}\right) + \tilde{P}\left(y^N - y\right). \tag{10}$$

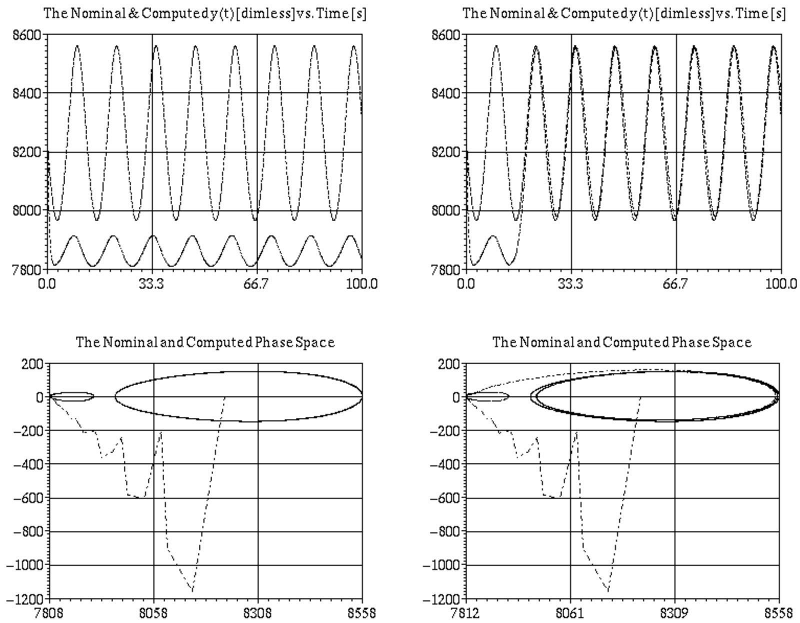

Figure 4
The 'trajectory' [1st row] and 'phase trajectory' [2nd row] tracking of the non-adaptive [left column], and the adaptive [right column] control.

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 of the time constant about T_{exp}. In order to realize (10) the rough initial model given in (9) was used with $\tilde{a}_{\mathrm{mod}} = -6\times10^6$ and $\tilde{b}_{\mathrm{mod}} = 10^5$ constant values. The control parameters were as follows ζ=0.08, and $D = \tilde{b}_{\mathrm{mod}}$ as defined in (7). Fig. 4 reveals that switching on the adaptivity at about 15 *s* from starting the control process the control becomes quite accurate in both the trajectory and the phase-trajectory tracking sense. In Fig. 5 the adaptive factor $s(t)$ and the process control $u(t)$ are described for the same parameter setting for a hypothetically noiseless and a hypothetically noisy case regarding the measurement of d^2y/dt^2. According to the 3rd row of the figure the supposed measurement noise was quite considerable in comparison with the actual values of of d^2y/dt^2. In spite of that the quality of the adaptive control remained quite good that testifies the *robustness* of the propesed method.

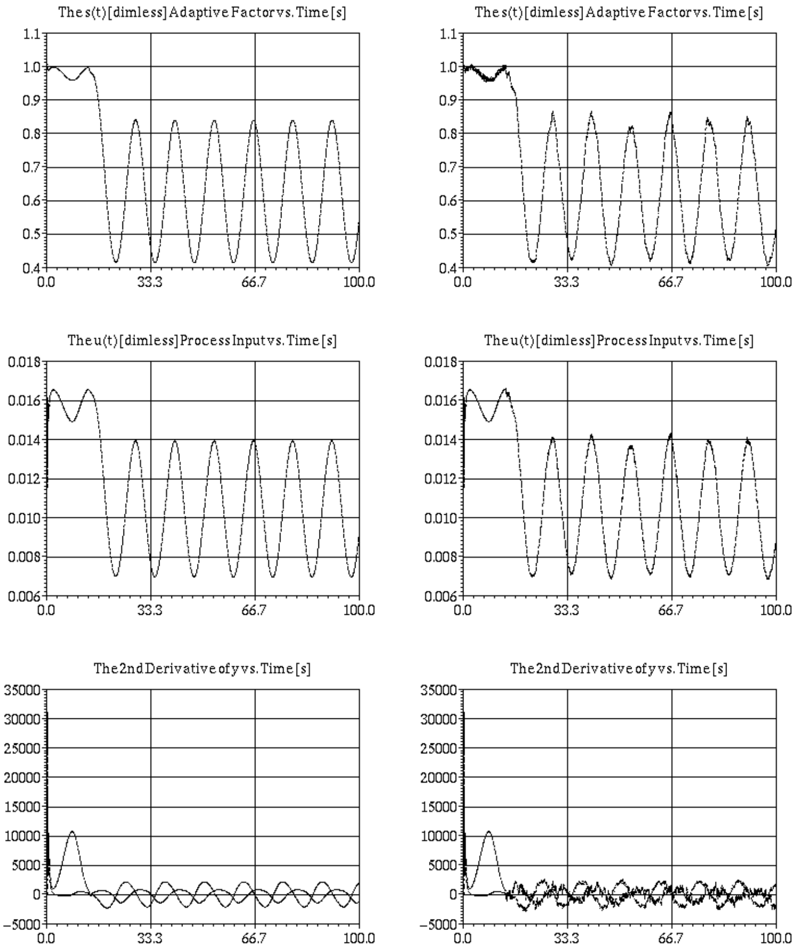

Figure 5

The adaptive factor *s* [1st row] and the control input *u* [2nd row] vs. time without measurement noise in d^2y/dt^2 [left column], and with evenly distributed random measurement noise restricted into the $[-10^3,+10^3]$ interval [in the non-adaptive initial part of the control $s(t)$ is only calculated but used]. The *desired* and the actual values of d^2y/dt^2 are given in the 3rd row.

Setting the control parameters used in the above simulations happened 'experimentally' by running several calculations numerically.

Regarding the proper value of ζ for the same $D = \tilde{b}_{\mathrm{mod}}$ *shifting parameter* various values were investigated according to Fig. 6 ζ=0.09 seems to be an optimal value at which the adaptation works quite quickly. On the basis of simple considerations (7) can result in *monotone* and in *fluctuating convergence* depending on the values of ζ and *D*. A plausible expalantion is that the contractivity of the mapping in (7) depends on ζ. For its small values $\zeta \leq\approx 0.09$ we have monotone convergence. At $\zeta \geq 0.09$ the mappimg still remans contractive but becomes fluctuatuing that can make it slower. (At higher values of ζ the contractivity can cease and the control algorithm may become divergent.)

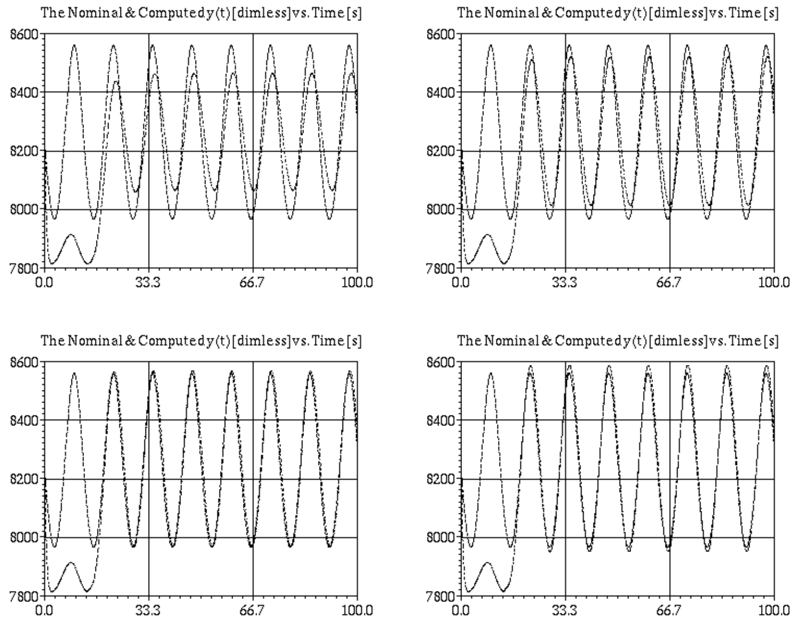

Figure 6

The operation of the dapative control for the settings of $D = \tilde{b}_{\mathrm{mod}}$ and ζ=0.04 [upper left], 0.06 [upper right], 0.09 [lower left], and 0.11 [lower right].

It also is evident from (7) that the slope of the function $g_{\zeta,D}$ also depends on *D*. Model calculations for its various values at ζ=0.09 are given in Fig. 7. It can well be seen that for the variation of the state variable **x** in the constrol task considered the fixed pair of ζ=0.09 and $D = \tilde{b}_{\mathrm{mod}}$ seems to be an approximately optimal setting.

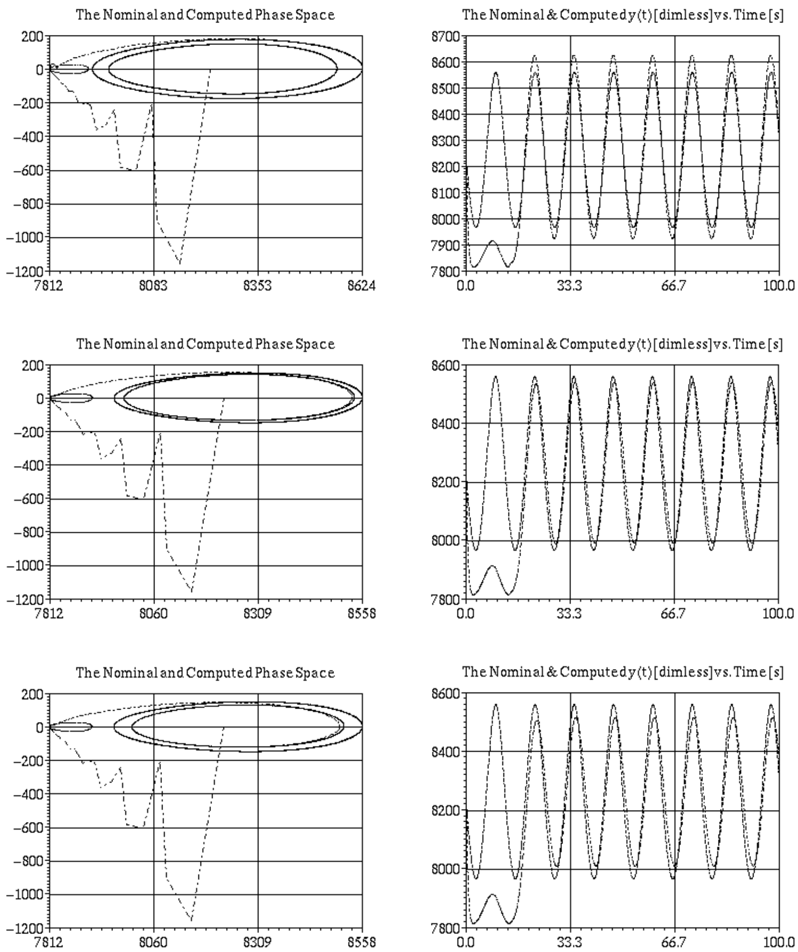

Figure 7

The dependence of the quality of the adaptive control on the value of the control parameter D=0.5× [1st row], 1.25× [2nd row], and 1.5× [3rd row] $\widetilde{b}_{\mathrm{mod}}$ at ζ=0.09: the phase trajectories [left column], and trajectory tracking [right column].

Conclusions

On the basis of a detailed numerical dynamic analysis of a quantitative mathematical model of the polymerization process considered It was shown that the process output is negative definite function of the process input (control signal) during the relaxation processes between the steady states caused by sudden jumps (steps) in the process input. On this basis an adaptive dynamic control was elaborated that used these two signals only. (The other internal degrees of freedom in dynamic coupling with the used ones remained hidden for the controller.)

The present approach was based on the *Extended Modification of the Renormalization Transformation* that was elaborated for negative definite SISO systems. This method contains two simple control parameters. The quality of the control was investigated via simulation from the points of view of its robustness with respect to setting its free parameters, and its sensitivity to the measurement noises. Robustness of the control with respect of these parameters means that no exact setting is needed for them. Their actual setting concerns the quality of the tracking of the control but does not influence the fact of the convergence.

It was concluded that at the time-scale of about 0.067 *s* sampling time the 'dynamics' of the controlled process could well be traced, and on the basis of a simple planning method quite accurate dynamic control was achieved.

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