Adaptive Control of a Polymerization Process

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Abstract: In this paper a simplified ARMAX-type (Autoregressive Moving Average model with eXternal input) adaptive control of a polymerization process approximately in its quasi-stationary limit is presented. This process 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 cannot be directly controlled: the desired output is nonlinear function of these quantities. In the present example only a single input variable is used for control purposes. In the paper detailed mathematical analysis of a quantitative model of the process is presented. It is concluded that at the time-scale commonly used in industrial control of such reactions (about 0.1-0.2 s sampling time) following the variation of the process input (control signal) the internal dynamics of the system achieves its stable stationary state with a rough approximation, therefore in the applied ARMAX-type control instead of the internal dynamics of the system the "dynamics" of the desired output is revealed, i.e. the controlled process is more or less similar to the concept of the "quasi-stationary processes" of Classical Thermodynamics. This fact sets certain limit to the available precision of the control if the desired control actions are faster than the characteristic variation of the internal dynamics. Improving this control requires far more detailed analysis and modelling of the process, and does not allow neglecting the dynamics of the internal degrees of freedom.

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. A discrete time model can be formulated in the form of a difference equation with an external input $\{u_k\}$ that usually is known quantity (Autoregressive Moving Average Model with eXternal input - ARMAX) [1]:

$$y_{k+1} = \sum_{s=0}^{N} a_s y_{k-s} + \sum_{w=0}^{M} b_w u_{k-w} \tag{1}$$

For instance, in the so-called Takagi-Sugeno fuzzy models the consequent parts are expressed by analytical expressions similar to (1) and they use some linear combinations of the (1)-type 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 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” 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 a complete model. 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. 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 the modification of the renormalization transformation extensively used in various fields of physics (e.g. [11]), 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 [12]. Though the convergence of the method in [11] can be guaranteed for a quite wide class of physical systems (e.g. for Classical Mechanical Systems), the latter one in [12] does not need so rigorous conditions, therefore in the sequel this one will be applied for the control of the chemical reaction considered as a paradigm.

2 Geometric Approach for Dynamic Systems

Consider a simple nonlinear causal Multiple Input – Multiple Output (MIMO) system described by the equation:

$$\mathbf{y}^{(n)}(t) = \mathbf{F}\left(\mathbf{y}^{(n-1)}(t), \mathbf{y}^{(n-2)}(t), \ldots, \mathbf{y}^{(0)}(t), \mathbf{f}(t)\right) \tag{2}$$

in which $\mathbf{f}(t)$ represents the external driving forces to be utilized for control purposes. Let us suppose that the time-derivatives can be approximated by certain finite element approach using time-resolution δt. To numerically estimate the n^{th} order time-derivatives at least $(n+1)$ discrete values has to be taken into account via considering their linear combination as

$$\mathbf{y}^{(n)}(t) \cong \sum_{s=0}^{n} \mathbf{c}_s(\delta t)\mathbf{y}(t - s\delta t) \tag{3}$$

in which the $\mathbf{c}_s$ coefficients depend on δt and can be chosen in various manners. We also note that the number of the coefficients may be somewhat greater that $(n+1)$, e.g. in the case of computing the central first derivatives we may use 3 points, too. Via rearranging (2) and using (3) the following *ambiguous representation* can be obtained:

$$\mathbf{y}(t) \cong \mathbf{\Phi}\left(\mathbf{y}(t-\delta t), \mathbf{y}(t-2\delta t), \ldots, \mathbf{y}(t-n\delta t), \mathbf{f}(t-\delta t)\right) \tag{4}$$

in which the actually used values are concentrated in the vicinity of the values of time t. Supposing that the array of the values $\mathbf{Y}_f := [\mathbf{y}(t-\delta t), \ldots, \mathbf{y}(t-n\delta t), \mathbf{f}(t-\delta t)]^T \neq \mathbf{0}$ in (4) can be replaced by a scalar product in ambiguous manner by an array $\mathbf{G}$ as

$$\mathbf{y}(t) = \mathbf{G}^T(t)\mathbf{Y}_f(t) \tag{5}$$

in which both the angle between $\mathbf{g}$ and $\mathbf{y}$ and the absolute value of $\mathbf{g}$ are not well defined. If the n^{th} derivative of $\mathbf{y}(t)$ is directly measurable similar ambiguous approximation can be constructed for $\mathbf{y}^{(n)}(t)$ as

$$\mathbf{y}^{(n)}(t) = \mathbf{g}^T(t)\mathbf{Y}_f(t). \tag{6}$$

Let us suppose that on the basis of some rough initial or preliminary model we can compute the appropriate control action $\mathbf{f}(t)$ and can store the $\mathbf{y}(t)$ values, too. It is evident that in the case of a time-invariant linear system $\mathbf{g}$ does not depend on t, therefore collecting sufficient information coded in the form of (6) leads to the system of linear equations that belong to the constant array $\mathbf{g}$ as

$$\begin{bmatrix} \mathbf{y}^{(n)}(t-\delta t) \\ \dots \\ \mathbf{y}^{(n)}(t-M\delta t) \end{bmatrix} = \begin{bmatrix} \mathbf{Y}_f^T(t-\delta t) \\ \dots \\ \mathbf{Y}_f^T(t-M\delta t) \end{bmatrix} \mathbf{g}. \tag{7}$$

Equation (7) has very simple and lucid geometric interpretation: the constant vector $\mathbf{g}$ is represented by time-varying or "floating" system of basis vectors $\mathbf{Y}_f(t-n\delta t)$ (n=1,…,M). If this set is linearly independent $\mathbf{g}$ can be reproduced as the linear combination of these vectors as

$$\mathbf{g} = \sum_{s=1}^{M} \mu_s(t)\mathbf{Y}_f^T(t-s\delta t) \tag{8}$$

In (8) it is naturally supposed that to a constant $\mathbf{g}$ for a floating system of basis vectors a floating or time-varying system of the $\mu_s(t)$ coefficients belongs in a special manner that they together can provide a constant vector. Let us suppose that we have two vectors $\mathbf{a}$ and $\mathbf{b}$ having known dot product with $\mathbf{g}$. The component of $\mathbf{b}$ in the orthogonal subspace of $\mathbf{a}$ can be expressed in the form of $\mathbf{b}_\perp = \mathbf{b} + \lambda\mathbf{a}$:

$$0 = \mathbf{a}^T\mathbf{b}_\perp = \mathbf{a}^T\mathbf{b} + \lambda\mathbf{a}^T\mathbf{a} \Rightarrow \lambda = \frac{-\mathbf{a}^T\mathbf{b}}{\mathbf{a}^T\mathbf{a}}. \tag{9}$$

Due to the linear property of the dot or "scalar" product the dot product of $\mathbf{b}_\perp$ with $\mathbf{g}$ can also be computed as

$$\mathbf{g}^T\mathbf{b}_\perp = \mathbf{g}^T\mathbf{b} + \lambda\mathbf{g}^T\mathbf{a}. \tag{10}$$

Now let us apply the following algorithm that is similar to the Gram-Schmidt orthogonalization with the exception of normalizing the vectors: remove the components in the direction of $\mathbf{Y}_f(t-\delta t)$ from $\mathbf{Y}_f(t-2\delta t)$,…, $\mathbf{Y}_f(t-M\delta t)$ with the method given in (9). Then the new set indexed with 2, 3,…, M-1 will be in the orthogonal subspace of $\mathbf{Y}_f(t-\delta t)$. Then take the 2^{nd} vector of the remaining set and subtract the components of the remaining ones in its direction, etc. while tracing the variation of the dot products according to (10). (To avoid numerical difficulties the components in the direction of very small vectors need no to be subtracted.) Since in the case of linear systems it is just enough to obtain sufficient information on the *independent directions* only, the approximately same direction of vectors $\mathbf{a}$ and $\mathbf{b}$ can be stated if

$$\left|\cos\varphi(\mathbf{a},\mathbf{b})\right| \cong \frac{\left|\mathbf{a}^T\mathbf{b}\right|}{\left|\mathbf{a}\right|\times\left|\mathbf{b}\right|+\varepsilon_1} \geq 1-\varepsilon_2 \,. \tag{11}$$

in which ε_1 and ε_2 are small positive numbers. Otherwise these vectors have *essentially different directions*. Via continuing the systematic observation further information can be obtained on **g** in the form of (6) as

$$\mathbf{y}^{(n)}(t+\delta t) = \mathbf{g}^T(t)\mathbf{Y}_f(t+\delta t). \tag{12}$$

Together with the information coded in (7) (12) is *redundant but free of contradiction* if **g** is exactly constant. In this case either (12) or one of the vectors in (7) can be dropped, replaced with the 1st vector in the set in (7), and the orthogonalization algorithm can be repeated. As a result the same constant **g** must be obtained by the use of this new set of basis vectors. If our system is *linear* but *not time-invariant* (7) and (12) are rather controversial than redundant because these vectors do not belong exactly to the same **g** since they were obtained in different time instances. A plausible means of contradiction resolution may be finding the vector in the closest direction of the last one in the sense of (11) since the remaining vectors convey less relevant information on the system's behavior in this direction. This vector can be replaced by the new information conveyed by (12). Then by executing the orthogonalization algorithm on the remaining set the "*obsolete information regarding the new direction*" can be removed and replaced by the fresh one. If our system is neither time-invariant nor linear then not only the directions but the absolute values of the vectors also influence its behavior. In this case the old vector closest to the new one in the sense of a norm can be dropped and replaced by the new one because the information mainly conveyed by it is "refreshed".

In the possession of some prescribed control strategy formulating the desired trajectory tracking with asymptotic convergence continuous tracking error is expected and the array **g** in (8) can be used for calculating the necessary control action instead of the rough initial model as

$$\mathbf{f}(t) = \mathbf{g}_M^{-1}\left\{\mathbf{y}^{(n)Desired}(t) - \begin{bmatrix}\mathbf{g}_1 & \ldots & \mathbf{g}_{M-1}\end{bmatrix}\begin{bmatrix}\mathbf{Y}_1 \\ \ldots \\ \mathbf{Y}_{M-1}\end{bmatrix}\right\} \tag{13}$$

in which the quadratic matrix $\mathbf{g}_M$ corresponds to those part of **g** in which the coefficients of **f**(t) are placed. In the special case of SISO or in the control of MIMO systems in which only one control signal is used and only one output is directly observed (13) is reduced to

$$f(t)=\left\{ y^{(n)Desired}(t)-\begin{bmatrix} g_1 & \dots & g_{M-1} \end{bmatrix}\begin{bmatrix} Y_1 \\ \dots \\ Y_{M-1} \end{bmatrix} \right\}\frac{1}{g_M} \tag{14}$$

in which the singularity avoidance can be solved in the following simple manner:

$$\frac{1}{x}\cong\frac{sign(x)}{|x|+\varepsilon_3} \tag{15}$$

with a small positive positive number ε_3.

3 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 [13]. In his Doctoral Thesis J. Madár applied a sophisticated approach based on Genetic Programming (GP) for identifying this reaction [14]. The aim of the present paper is to investigate a more simple temporal identification approach for this system. According to [13] the model considered is:

$$\begin{aligned} &\dot{x}_1 = A(B-x_1)-Cx_1x_2^{1/2}, \quad \dot{x}_2 = Du-Ex_2 \\ &\dot{x}_3 = FCx_1x_2^{1/2}+Gx_2-Hx_3, \quad \dot{x}_4 = Ix_1x_2^{1/2}-Jx_4 \\ &y := \frac{x_4}{x_3} \end{aligned} \tag{16}$$

in which the state variables $x_1, \dots, x_4$ 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, u is the *dimensionless volumetric flow rate of the initiator*. The constants in (16) 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 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 positive numbers or zero. It is easy to see that for a constant process input u (16) yields a *stationary solution* in which the time-derivatives of the state variables are equal to zero:

$$x_2^{stac}=\frac{Du}{E},\quad x_1^{stac}=\frac{AB}{A+C\sqrt{\frac{Du}{E}}},$$
$$x_3^{stac}=\frac{F}{H}\frac{AB}{A+C\sqrt{\frac{Du}{E}}}\sqrt{\frac{Du}{E}}+\frac{G}{H}\frac{Du}{E}, \tag{17}$$
$$x_4^{stac}=\frac{I}{J}\frac{AB}{A+C\sqrt{\frac{Du}{E}}}\sqrt{\frac{Du}{E}}$$

in which the sequence of the quantities corresponds to the easiest way of the calculation. Due to the positive nature of u and the constants in (17) it is evident that the stationary solutions are positive numbers. The stability of the stationary solution can be proved via the perturbation calculus as follows: an infinitesimally small variation in the process input δu is supposed, and the time-dependent terms are considered as small perturbations on the constant stationary states as

$$x_i(t)=x_i^{stac}+\delta x_i(t),\quad i=1,2,3,4\,. \tag{18}$$

Via replacing (18) into (16) and keeping only the 0th and the 1st order terms in the perturbations the first order system of differential equations of constant coefficients can be obtained:

$$\begin{bmatrix}\delta\dot{x}_1\\ \delta\dot{x}_2\\ \delta\dot{x}_3\\ \delta\dot{x}_4\end{bmatrix}=\begin{bmatrix}-A-C\sqrt{x_2^{stac}} & -C\frac{x_1^{stac}}{2\sqrt{x_2^{stac}}} & 0 & 0\\ 0 & -E & 0 & 0\\ F\sqrt{x_2^{stac}} & G+F\frac{x_1^{stac}}{2\sqrt{x_2^{stac}}} & -H & 0\\ I\sqrt{x_2^{stac}} & I\frac{x_1^{stac}}{2\sqrt{x_2^{stac}}} & 0 & -J\end{bmatrix}\begin{bmatrix}\delta x_1\\ \delta x_2\\ \delta x_3\\ \delta x_4\end{bmatrix}+\begin{bmatrix}0\\ D\delta u\\ 0\\ 0\end{bmatrix}. \tag{19}$$

In the special case in which $\delta u=0$ and the $\delta x_i(0)\neq 0$ initial perturbations are finite values (19) corresponds to exponentially damped perturbations if the eigenvalues of the big matrix in it are negative numbers. In Fig. 1 the stationary output is described versus the process control, as well as the eigenvalues of the matrix in (19) in an investigated case. The stationary solutions evidently were stable in the cases numerically investigated. The $\delta u\neq 0$ constant case with $\delta x_i=0$ initial errors corresponds to an infinitesimal constant modification in the process input to which evidently finite (infinitesimally small) $\delta x_i\neq 0$ state modifications belong (the concept of the "quasi-stationary process" in Classical Thermodynamics). Really, if the variation of u is far slower than that of the internal dynamics of the system the modification of the state-variables are properly mapped to the variation of u

according to Fig. 1 when the transients are completely damped. In the sequel the adaptive control of this system is investigated.

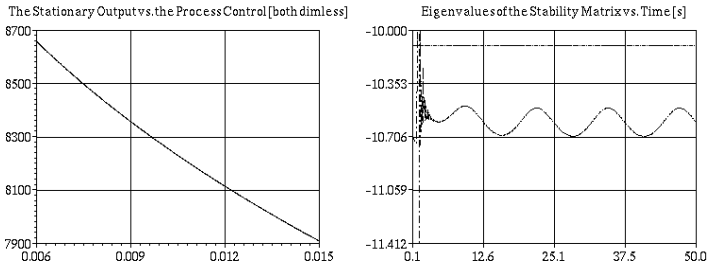

Figure 1

The stationary process output vs. the constant process input (left side), and the eigenvalues of the matrix in (19) in the range investigated (right side)

4 Simulation Results

In the forthcoming simulation examples δt=0.04 *s* and 0.1 *s* sampling times were supposed for the controller, while the numerical integration of the transients happened with δt_{int}=0.0001 *s* step length. For the process output the following "kinematic" restriction was prescribed:

$$\dot{y}^{Des} = \dot{y}^{Nom} + P\left(y^{Nom} - y\right). \tag{20}$$

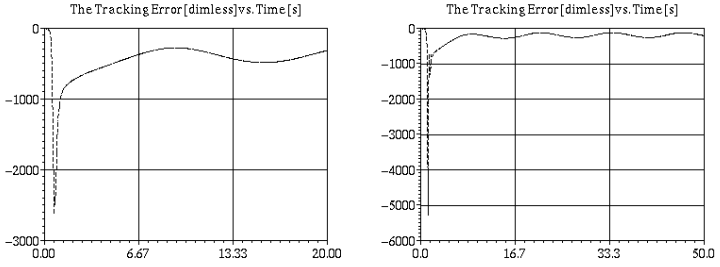

Figure 2

The nominal and the simulated stationary process output vs. time [*s*] for the δt=0.04 *s* (left side), and the δt=0.10 *s* (right side) sampling times in the case of an "*almost quasi-stationary*" motion

In Fig. 2 the tracking properties of the controller are given for "quasi-stationary" cases. It is obvious that the δt=0.04 *s* sampling time is not enough for tracking the consequences of the transients, and increasing it to δt=0.10 *s* improves the

tracking precision. For substantiating the plausible supposition that in the case of a quasi-stationary motion the ARMAX-type controller "identifies" rather the properties of the nominal motion than that of the dynamics of the system under control in Fig. 3 the 1st three identified components of the vector **g** in (8) are described in both cases.

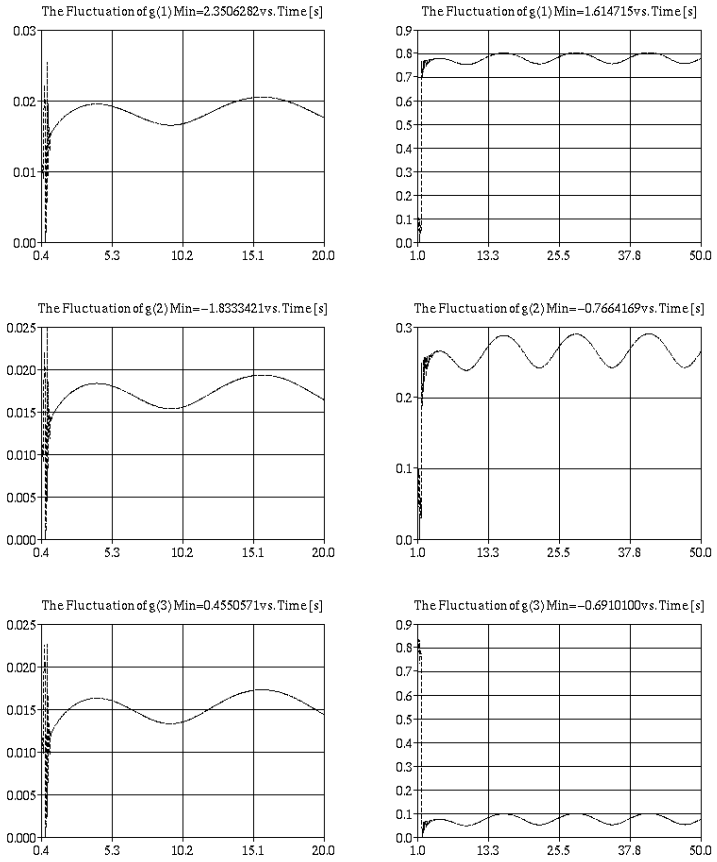

Figure 3

The variation of the 1st three identified components of **g** vs. time [*s*] for the δt=0.04 *s* (left side), and the δt=0.10 *s* (right side) sampling time in the case of the "*almost quasi-stationary*" motion

The identified components of **g** in Fig. 3 virtually vary almost precisely according to the frequency of the "nominal motion" as given in Fig. 2. A vector **g** of four components roughly corresponds to a three points based finite elements approximation of the velocity and a single excitation point based approach (like in the case of an inhomogeneous differential equation). Consequently the value of

the sampling time concerns the absolute values in **g**. Fig. 4 reveals similar periodic behaviour in the 4th component of **g** pertaining to the "excitation" or "process control" signal $u(t)$.

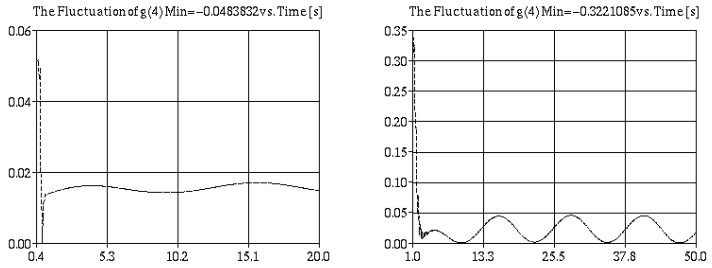

Figure 4

The variation of the 4th identified component of **g** vs. time [*s*] for the δt=0.04 *s* (left side), and the δt=0.10 *s* (right side) sampling time in the case of the "*almost quasi-stationary*" motion

It is worth noting in the case of the different sampling times the nominal motion had the same frequency, and the simulations were carried out for 500 steps. Due to the proportional error-compensating term in (20) further increase in the sampling time at the same nominal frequency leads to too big discrete jump in the feedback that may result in loosing the control's stability.

Conclusions

In this paper a special, simplified ARMAX-type adaptive control was applied for controlling a polymerization process. This process served as an appropriate paradigm of multivariable dynamic systems of strong non-linear coupling between different internal dynamic degrees of freedom. In the example these quantities were not directly controlled: the desired output was nonlinear function of these quantities, and only a single input variable was used for control purposes. On the basis of a detailed mathematical analysis of a quantitative model of the process it was 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, therefore in the applied ARMAX-type control instead of the internal dynamics of the system rather the "dynamics" of the desired output was revealed. This meant that the controlled process was more or less similar to the concept of the "quasi-stationary processes" of Classical Thermodynamics. This fact in general sets certain limit to the available precision of the control if the desired control actions are faster than the characteristic variation of the internal dynamics of the system. Improving this control requires far more detailed analysis and modelling of the process, and does not allow neglecting the dynamics of the internal degrees of freedom.

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