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Neuro-fuzzy Control of a Chemical Reactor with Uncertainties

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Abstract: This work deals with the design and application of a neuro-fuzzy control of a chemical reactor. The reactor is exothermic one. There are two parameters with only approximately known values in the reactor. These parameters are the reaction enthalpies. Because of the presence of uncertainty in the continuous stirred tank reactor, the robust output feedback is designed. The simulation results confirm that fuzzy control is one of the possibilities for successful control of chemical reactors.

1. INTRODUCTION

It is well known that the control of chemical reactors often represents very complex problems (Luyben 2007), (Molnár et al. 2002). Continuous stirred tank reactors (CSTRs) are often used plants in chemical industry and especially exothermic CSTRs are very interesting systems from the control viewpoint (Bequette 1991). The dynamic characteristics may exhibit a varying sign of the gain in various operating points, the time delay as well as non-minimum phase behaviour. Various types of disturbances also affect operation of chemical reactors, operation of chemical reactors is corrupted by many different uncertainties. Some of them arise from varying or not exactly known parameters, as e.g. reaction rate constants, reaction enthalpies or heat transfer coefficients (Antonelli and Astolfi 2003). All these problems can cause poor control response or even instability of classical closed-loop control systems.

Effective control of CSTRs requires application of some of advanced methods, as e. g. robust control (Gerhard et al. 2004), (Tlacuahuac et al. 2005). Robust control has grown as one of the most important areas in modern control design since works by (Doyle 1981), (Zames 1983) and many others.

Soft computing is a collection of methodologies like fuzzy system, neural networks and genetic algorithm, designed to tackle imprecision and uncertainty involved in a complex nonlinear system. Recent reviews on soft computing around the world (Dote and Ovaska 2001) indicate that the number of soft computing based engineering applications is increasing.

Fuzzy system has been known to provide a framework for handling uncertainties and imprecision by taking linguistic information from human experts. Fuzzy logic controllers have the advantages over the conventional controllers: they are cheaper to develop, they cover a wider range of operating conditions, and they are more readily customizable in natural language terms. FLCs have been implemented successfully in a variety of applications (Shapiro 2004), (Hayward and Davidson 2003), (Peri and Simon 2005).

Fuzzy controllers are more robust than PID controllers because they can cover a much wider range of operating conditions than PID can, and can operate with noise and disturbances of different nature. Given the dominance of conventional PID control in industrial applications, it is significant both in theory and in practice if a controller can be found that is capable of outperforming the PID controller with comparable ease of use. Some of PID fuzzy controllers are quite close to this aim (Ying 2000). The simplest and most usual way to implement a fuzzy controller is to realize it as a computer program on a general purpose computer.

One popular soft computing method is neuro-fuzzy technique which is a hybrid combination of artificial neural networks (ANN) and fuzzy inference system (FIS). Adaptive Network based Fuzzy Inference System (ANFIS) (Jang 1993), (Jang et al. 1997) is such a neuro-fuzzy technique. A clustering algorithm partitions a data set into several groups such that the similarity within a group is larger than among groups (Jang et al. 1997). The idea of data grouping, or clustering, is simple in its nature and is close to the human way of thinking (Jain and Dubes 1988). A more recent overview can be found in a collection of (Bezdek and Pal 1992), (Backer 1995).

2. FUZZY CONTROL

Classic control theory is usually based on mathematical models which describe the behaviour of the process under consideration. The main aim of fuzzy control is to simulate a human expert (operator), who is able to control the process by translating the linguistic control rules into a fuzzy set theory.

In 1965 Lotfi A. Zadeh introduced fuzzy sets, where a more flexible sense of membership is possible. The past few years have witnessed a rapid growth in the use of fuzzy logic controllers for the control of processes that are complex and badly defined. Most fuzzy controllers developed till now have been of the rule-based type (Driankov et al. 1993), where the rules in the controller attempt to model the operator´s response to particular process situations. An alternative approach uses fuzzy or inverse fuzzy model in process control (Babuška et al. 1995), (Jang 1995) because it is often much easier to obtain information on how a process responds to particular inputs than to record how, and why, an operator responds to particular situations. A review of the work on fuzzy control has been presented by Lee (Lee 1990).

Design of a simple fuzzy controller can be based on a three-step design procedure that builds on PID control: start with a PID controller, insert an equivalent, linear fuzzy controller and make it gradually nonlinear.

A fuzzy controller (Fig. 1) can include empirical rules, and that is especially useful in operator controlled plants. Take e.g. a typical fuzzy controller:

- if error is negative and change in error is negative then output is negative big
- if error is negative and change in error is zero then output is negative medium.

The collection of rules is called a rule base. The computer is able to execute the rules and compute a control signal depending on the measured inputs error and change in error. The inputs are most often hard or crisp measurements from some measuring equipment. A dynamic controller would have additional inputs, for example derivatives, integrals, or previous values of measurements backwards in time.

The block fuzzification converts each piece of input data to degrees of membership by a lookup in one or several membership functions. The rules may use several variables both in the condition and the conclusion of the rules. Basically a linguistic controller contains rules in the if-then format, but they can be presented in different formats.

The resulting fuzzy set must be converted to a number that can be sent to the process as a control signal. This operation is called defuzzification. There are several defuzzification methods. Output scaling is also relevant.

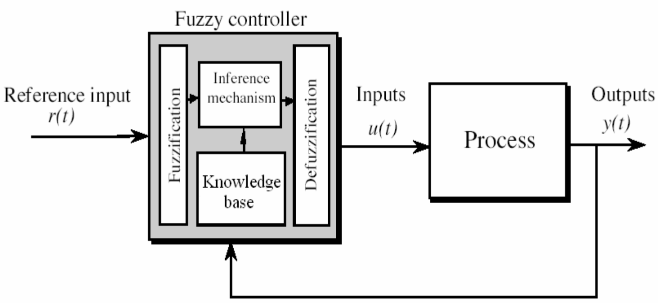

Fig. 1. Fuzzy control (Passino and Yurkovich 1998)

3. ADAPTIVE NETWORK BASED FUZZY INFERENCE SYSTEM (ANFIS)

The output sets can often be linear combinations of the inputs, or even a function of the inputs. The developed Fuzzy Logic Toolbox for the software package Matlab implements one of the hybrid schemes known as the ANFIS. ANFIS represents a Sugeno-type fuzzy system. Suppose the rule base of a Sugeno - Takagi fuzzy system as follows (Nauck et al. 1977), (Takagi et al. 1985):

$$\text{if } x_1 \text{ is } A_i \text{ and } x_2 \text{ is } B_i$$
$$\text{then } y = p_i x_1 + q_i x_2 + r_i,\ i = 1, ..., N \tag{1}$$

The if-parts (antecedents) of the rules describe fuzzy regions in the space of input variables error e, its derivative de and the then-parts (consequents) are functions of the inputs, usually linear with consequent parameters p_i, q_i, r_i, y is an output variable, A_i, B_i are fuzzy sets.

ANFIS represents a useful neural network approach for the solution of function approximation problems. Data driven procedures for the synthesis of ANFIS networks may be based on the subtractive clustering technique (Chiu 1994) of the input-output space of a training set of numerical samples of the unknown function to be approximated.

In the ANFIS architecture, FIS is described in a layered, feedforward network structure (Fig. 6.). The parameters in layer 1 are called premise parameters and they are adjustable. The second layer represents the *T*-norm operators that combine the possible input membership grades in order to compute the firing strength of the rule. In the basic ANFIS method these parameters are not adjustable. The third layer implements a normalisation function to the firing strengths producing normalised firing strengths. The fourth layer represents the consequent parameters that are adjustable. The fifth layer represents the aggregation of the outputs performed by weighted summation. This is not adjustable.

3.1 Subtractive clustering

Subtractive clustering method is a method which extracts rules from supplied input-output training data. The idea of fuzzy clustering is to divide the data space into fuzzy clusters, each representing one specific part of the system behavior. After projecting the clusters onto the input space, the antecedent parts of the fuzzy rules can be found. The consequent parts of the rules can then be simple functions. In this way, one cluster corresponds to one rule of the TSK model. Several clustering methods are well known (Chiu 1994), (Yager and Filev 1994).

Let us consider a collection of n data points $\{x_1, x_2, ..., x_n\}$ in an M dimensional space. Each data point is a candidate for cluster centers, a density measure at data point $\mathbf{x}_i$ is defined as

$$P_k = \sum_{j=1}^{N} exp\left(-\alpha \left\| x_k - x_j \right\|^2\right) \tag{2}$$

where $\alpha = \dfrac{\gamma}{(r_a)^2}$, P_k is the new potential-value of each examined point, α is the weight between i-data to j-data, x is the data point, γ is variables (commonly set 4), r_a is a cluster radius, it is a positive constant that represents the radius of data neighborhood.

A data point will have a high density value if it has many neighboring data points. The first cluster center x_{c1} is chosen as the point having the largest density value P_{c1}. Next, the density measure of each data point x_i is revised as follows:

$$P'_k = P_k - P_{c1}\exp\left(-\beta\left\|x_k - x_{c1}\right\|^2\right) \tag{3}$$

where $\beta=\gamma/(r_b)^2$, $r_b = r_a\eta$, r_b is a positive constant which defines a neighborhood that has measurable reductions in density measure. Therefore, the data points near the first cluster center x_{c1} will have significantly reduced density measure. P_{c1} is the new potential-value data as cluster centre, β is the weight of i-data to cluster centre, η is the quash factor, usually set 1,5, r_i is the distance between cluster centre.

When the potential of all data points have been revised according to (3), the data point with highest remaining potential is selected as the second cluster center. We then further reduce the potential of each data point according to their distance to the second cluster center. The process is repeated until the potential of the points reaches the stopping criterion $P'_k < \varepsilon P_{c1}$, where ε is the reject ratio, usually set 0,15.

4. SIMULATION AND RESULTS

4.1 *Chemical reactor*

Consider a continuous-time stirred tank reactor (CSTR) with the first order irreversible parallel exothermic reactions according to the scheme $A \xrightarrow{k_1} B$, $A \xrightarrow{k_2} C$, where B is the main product and C is the side product. The dynamic mathematical model of the reactor is obtained by mass balances of reactants, enthalpy balance of the reactant mixture and enthalpy balance of the coolant. Assuming ideal mixing in the reactor and other usual simplifications (Ingham et al. 1994), (Vasičkaninová and Bakošová 2006), the simplified nonlinear dynamic mathematical model of the chemical reactor consists of five differential equations

$$\frac{dc_A}{dt} = \frac{q}{V}c_{Av} - \frac{q}{V}c_A - k_1c_A - k_2c_A \tag{4}$$

$$\frac{dc_B}{dt} = \frac{q}{V}c_{Bv} - \frac{q}{V}c_B + k_1c_A \tag{5}$$

$$\frac{dc_C}{dt} = \frac{q}{V}c_{Cv} - \frac{q}{V}c_C + k_2c_A \tag{6}$$

$$\frac{dT}{dt} = \frac{q}{V}T_v - \frac{q}{V}T - \frac{Ak}{V\rho c_p}\left(T - T_c\right) - \frac{h_1k_1 + h_2k_2}{\rho c_p}c_A \tag{7}$$

$$\frac{dT_c}{dt} = \frac{q_c}{V_c}T_{vc} - \frac{q_c}{V_c}T_c + \frac{Ak}{V_c\rho_c c_{pc}}\left(T - T_c\right) \tag{8}$$

with initial conditions $c_A(0)$, $c_B(0)$, $c_C(0)$, $T(0)$, $T_c(0)$. The reaction rate coefficients are non-linear functions of the reaction temperature being defined by the Arrhenius relations

$$k_i = k_{i0}e^{-\frac{E_i}{RT}},\ i = 1,2 \tag{9}$$

Here, c are concentrations, T are temperatures, V are volumes, ρ are densities, c_p are specific heat capacities, q are volumetric flow rates, h are reaction enthalpies, A is the heat transfer area, k_i is the heat transfer coefficient, k_{i0} is the pre-exponential factor, E is the activation energy and R is the universal gas constant. The subscript c denotes the coolant and the superscript s denotes the steady-state values in the main operating point.

The values of constant parameters and steady-state inputs of the chemical reactor are summarized in Table 1. Model uncertainty of the over described reactor follows from the fact that there are two physical parameters in this reactor, the reaction enthalpies, which values are known within following intervals (Table 2). The nominal values of these parameters are mean values of theirs intervals.

Table 1. Constant parameters and steady-state inputs of the chemical reactor

Variable	Unit	Value
q	$m^3 min^{-1}$	0,015
V	m^3	0,23
V_C	m^3	0,21
ρ	$kg\ m^{-3}$	1020
ρ_C	$kg\ m^{-3}$	998
c_p	$kJ\ kg^{-1}\ K^{-1}$	4,02
c_{pc}	$kJ\ kg^{-1}\ K^{-1}$	4,182
A	m^2	1,51
k	$kJ\ m^{-2}\ min^{-1}\ K^{-1}$	42,8
k_{10}	min^{-1}	$1,55\times10^{11}$
k_{20}	min^{-1}	$4,55\times10^{25}$
E_1/R	K	9850
E_2/R	K	22019
c_{Av}	$kmol\ m^{-3}$	4,22
c_{Bv}	$kmol\ m^{-3}$	0
c_{Cv}	$kmol\ m^{-3}$	0
T_v	K	328

T_{vc}	K	298
q^s_c	$m_3\ min^{-1}$	0,004
T^s	K	363,61
T^s_c	K	350,15
c^s_A	kmol m^{-3}	0,4915
c^s_B	kmol m^{-3}	2,0042
c^s_C	kmol m^{-3}	1,7243

Table 2. Uncertain parameters of the chemical reactor

Variable	Unit	Value
$-h_{1min}$	kJ $kmol^{-1}$	$8{,}4\times10^4$
$-h_{1max}$	kJ $kmol^{-1}$	$8{,}8\times10^4$
$-h_{2min}$	kJ $kmol^{-1}$	$1{,}62\times10^4$
$-h_{2max}$	kJ $kmol^{-1}$	$2{,}02\times10^4$

4.3 Neuro-fuzzy controller of the chemical reactor

In this paper, ANFIS and subtractive clustering method were used to design fuzzy controller. The design procedure is conducted in two stages: first subtractive clustering is applied to extract fuzzy model from experimental data; then ANFIS is applied to improve the fuzzy model performance.

Sugeno-type neuro-fuzzy inference system was generated in the form:

$$\begin{aligned} &if\ e \text{ is } A_i \text{ a } \frac{de}{dt} \text{ is } B_i \text{ a } \int e \text{ is } C_i \\ &then\ f_i = p_i e + q_i \frac{de}{dt} + r_i \int e + s_i, \quad i = 1,\ldots,8 \end{aligned} \tag{10}$$

where e is the control error, p_i, q_i, r_i, s_i are consequent parameters. The symmetric Gaussian function (*gaussmf* in MATLAB) (11) was chosen as the membership function. The Gaussian function μ depends on two parameters σ and c as it is seen in (8), where x represents e, de/dt *or* $\int e$.

$$\mu(x;\sigma,c) = e^{\left[\frac{-(x-c)^2}{2\sigma^2}\right]} \tag{11}$$

The parameters σ and c for *gaussmf* are listed in the Table 3. For obtaining of these parameters, it was necessary to have the input data sets. These data were obtained by simulation of experimental PID controllers. The consequent parameters in the control input rule (10) are listed in Table 4. Figure 2 demonstrates the Takagi-Sugeno fuzzy inference system. Figure 3 shows the structure of Anfis.

Table 3. Parameters of the Gaussian curve membership functions

e		de		$\int e$	
σ_i	c_i	σ_i	c_i	σ_i	c_i
2,91	-4,72	0,44	-0,37	23,9	-56,33
2,95	2,71	0,50	0,79	23,9	0,0013

Table 4. Consequent parameters

p_i	q_i	r_i	s_i
$-3{,}1\times10^{-3}$	$-1{,}6\times10^{-4}$	$-6{,}7\times10^{-3}$	$8{,}3\times10^{-3}$
$-3{,}1\times10^{-3}$	$-2{,}6\times10^{-4}$	$-5{,}4\times10^{-3}$	$2{,}4\times10^{-3}$
$-2{,}9\times10^{-3}$	$-1{,}5\times10^{-4}$	$-6{,}1\times10^{-3}$	$5{,}6\times10^{-3}$
$-3{,}3\times10^{-3}$	$-2{,}5\times10^{-4}$	$-7{,}0\times10^{-3}$	$3{,}9\times10^{-3}$
$-3{,}2\times10^{-3}$	$-2{,}6\times10^{-4}$	$-6{,}7\times10^{-3}$	$2{,}3\times10^{-3}$
$-3{,}3\times10^{-3}$	$-2{,}2\times10^{-4}$	$-7{,}0\times10^{-3}$	$4{,}8\times10^{-3}$
$-3{,}1\times10^{-3}$	$-2{,}6\times10^{-4}$	$-6{,}6\times10^{-3}$	$3{,}4\times10^{-3}$
$-3{,}3\times10^{-3}$	$-2{,}2\times10^{-4}$	$-6{,}3\times10^{-3}$	$4{,}0\times10^{-3}$

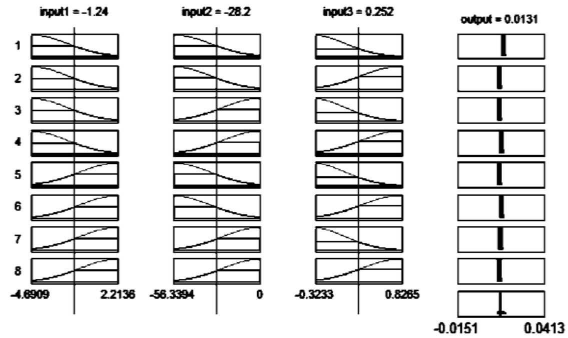

Fig. 2. Fuzzy inference system

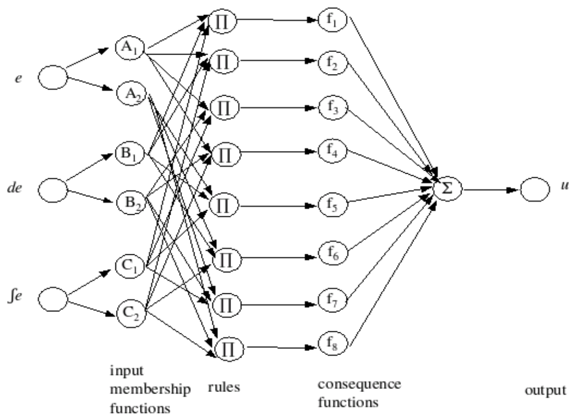

Fig. 3. Structure of Anfis

4.4 Control of the chemical reactor

The reactions in the described reactor are exothermic ones and the heat generated by the chemical reactions is removed by the coolant in the jacket of the tank. The measured output is temperature of the reaction mixture T, the coolant flow rate q_c is chosen as the control input. The control objective is to keep the temperature of the reacting mixture close to a desired value.

The steady state behaviour of the chemical reactor with nominal values and also with 4 combinations of minimal and maximal values of 2 uncertain parameters was studied at first. The maximal concentration of the main product B is obtained by temperature T=355 K (Fig. 4).

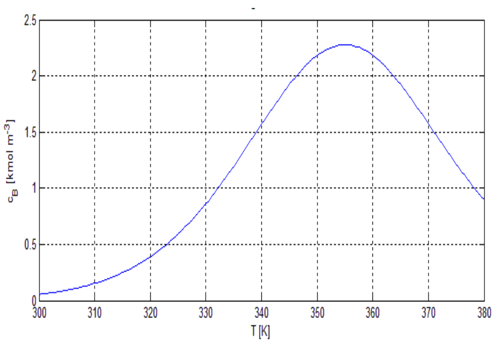

Fig. 4. Concentration of the main product B in the dependence on the T

The open-loop behaviour of the reactor was also studied. Simulation results obtained for the nominal model and also for 4 vertex systems are shown in Figure 5, 0 – nominal system, 1 – h_{1min}, h_{2min}, 2 – h_{1max}, h_{2max}, 3 – h_{1max}, h_{2min}, 4 – h_{1min}, h_{2max}.

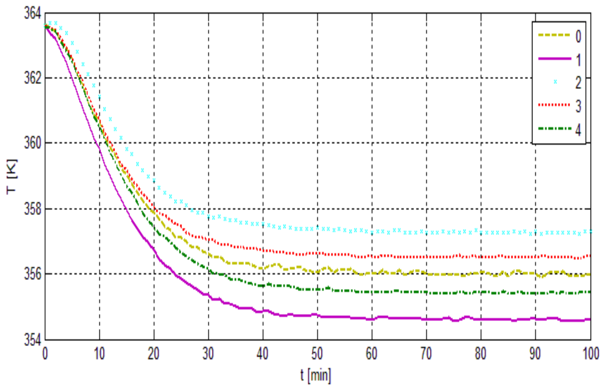

Fig. 5. Open-loop response of the CSTR: 0 - nominal system, 1, 2, 3, 4 - vertex systems

In Figure 6 the neuro-fuzzy control of the reacting mixture temperature and the reference trajectory obtained for the nominal model and for 4 vertex systems are shown. The control inputs are presented in Figure 7. The controller is fast and the overshoots are minimal.

In praxis, it is necessary to work with noisy signals, the white noise was added to the controlled output. Figures 8, 9 present the simulation results of the fuzzy control of the chemical reactor in the case when disturbances affect the controlled process. Disturbances were represented by temperature changes in the feed temperature of the reaction mixture. Following disturbances were loaded: T decreased by 5 K at t=200 min and increased by 10 K at t=200 min.

The neuro-fuzzy PID controller attenuates disturbances very fast and the overshoots caused by disturbances are minimal.

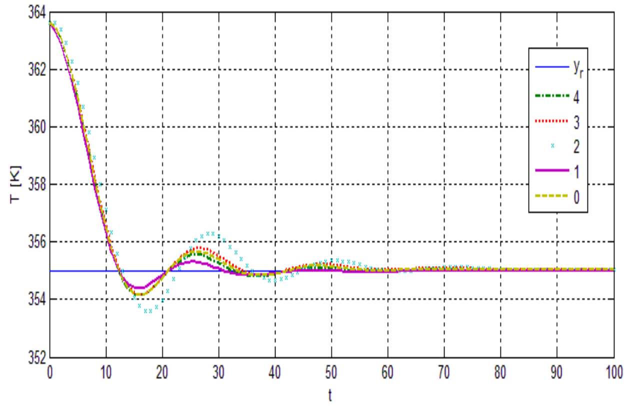

Fig. 6. Control of the CSTR: 0 - nominal system, 1, 2, 3, 4 - vertex systems

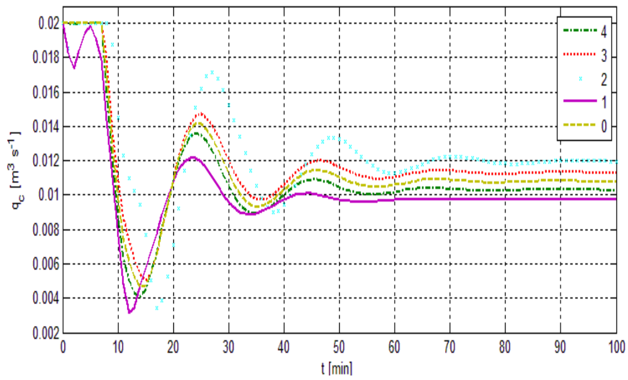

Fig. 7. Control inputs to the CSTR: 0 - nominal system, 1, 2, 3, 4 - vertex systems

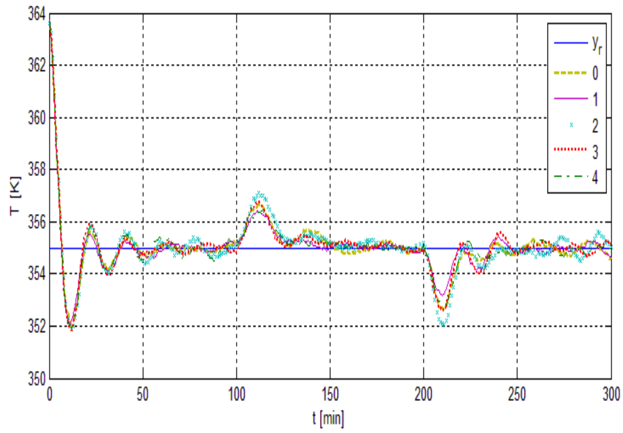

Fig. 8. Control of the CSTR with disturbances and noisy signals: 0 - nominal system, 1, 2, 3, 4 - vertex systems

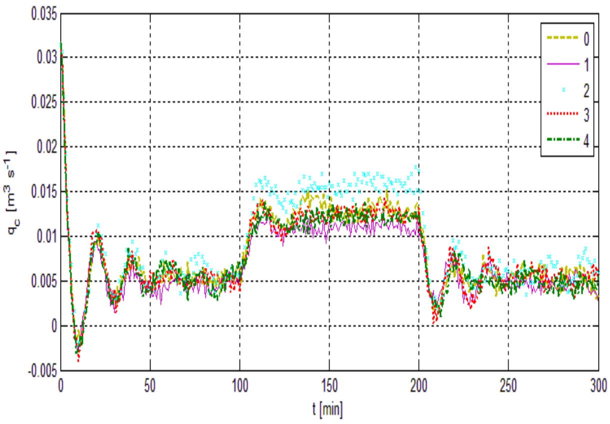

Fig. 9. Control inputs to the CSTR with disturbances and noisy signals: 0 - nominal system, 1, 2, 3, 4 - vertex systems

5. CONCLUSIONS

In this paper, the neuro-fuzzy control is applied to the exothermic CSTR with uncertain parameters. Simulations confirmed that robust neuro-fuzzy controllers can be successfully used for control of CSTRs with uncertainties and disturbances, even though CSTRs are very complicated systems from the control point of view. All simulations were done using MATLAB.

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