Korean J. Chem. Eng., **27**(1), 19-31 (2010)
DOI: 10.1007/s11814-009-0347-8

Double-command fuzzy control of a nonlinear CSTR

Morteza Mohammadzaherf and Lei Chen

Mechanical Engineering School, University of Adelaide, Adelaide 5005, South Australia
(Received 15 April 2009 • accepted 27 July 2009)

Abstract - In this research, double-command control of a nonlinear chemical system is addressed. The system is a stirred tank reactor; two flows of liquid with different concentrations enter the system through two valves and another flow exits the tank with a concentration between the two input concentrations. Fuzzy logic was employed to design a model-free double-command controller for this system in the simulation environment. In order to avoid output chattering and frequent change of control command (leading to frequent closing-opening of control valves, in practice) a damper rule is added to the fuzzy control system. A feedforward (steady state) control law is also derived from the nonlinear mathematical model of the system to be added to feedback (fuzzy) controller generating transient control command. The hybrid control system leads to a very smooth change of control input, which suits real applications. The proposed control system offers much lower error integral, control command change and processing time in comparison with neuro-predictive controllers.

Key words: Fuzzy Control, Hybrid Control, CSTR, Nonlinear System, Steady State Control

INTRODUCTION

Catalytic continuous stirred tank reactors (CSTR)s have been extensively used as a benchmark for testing different control systems. These systems are multi-input and multi-output and may be highly nonlinear. Self-tuning PIDs [1,2] robust controllers [3], adaptive-like control systems [4], and different kinds of nonlinear predictive controllers [5,6] have been successfully tested on this class of chemical systems. The CSTR is also known as an outstanding example for the application of neuro-predictive controllers [7], which are a sub-class of nonlinear predictive controllers. Moreover, fuzzy logic controllers are used in the control of CSTRs to generate either the control command directly [8,9] or control command increments [10,11]. As well as improving the performance; other aims achieved by the application of fuzzy control systems on CSTRs are stability guarantee [8,12] and disturbance rejection [13,14].

In this paper, at first, successful control of a non-thermic CSTR by neuro-predictive technique is reported. In this test, the flow mass rate of one of two entering flows is subject to adjustment in order to control outlet concentration of the tank Although, this problem is known as a good example for neuro-predictive control [7,15]. This technique worked both ineffectively (in terms of offering improper performance) and inefficiently (in terms of needing heavy computation) when it was tried for double-command control (to adjust the mass rate of both inlet flows). This paper then presents a hybrid control system designed to adjust the flow rates of both entering flows simultaneously. In the presented control system, the control commands are the sum of a transient control command whose increments are generated by a non-model-based fuzzy logic controller and a steady state control command generated by a set-point dependent control law. Finally, the control system was tested in simulation environment. In order that the results are applicable in practice, the "input constancy" is particularly addressed; that is, the proposed control system is designed to reduce the change of control inputs as well as the error.

THE UTILIZED FUZZY INFERENCE SYSTEM

In this research, a non-weighted first-order Sugeno type fuzzy inference system, with AND connectors, is used as the fuzzy controller. A schematic of such a system is shown in Fig. 1. Each fuzzy rule includes two main parts: antecedent and consequent. Antecedents contain linguistic (fuzzy) values with membership functions. A 'membership function' is a function which receives the crisp (numeric) value of a variable (e.g., 25 °C) and returns another number in the range of [0,1], namely 'membership grade'. As a result, in each rule, the number of membership grades equals the number of fuzzy values in the antecedent. All these membership grades (in the range of 0 and 1) pass through a function, namely T-norm The output of the T-norm is the fire strength of the rule:

fire strength of rule (w_i)=Tnorm (all membership grades), (1)

The fire strengths of rules (w_i) are the outcome of this step. In a

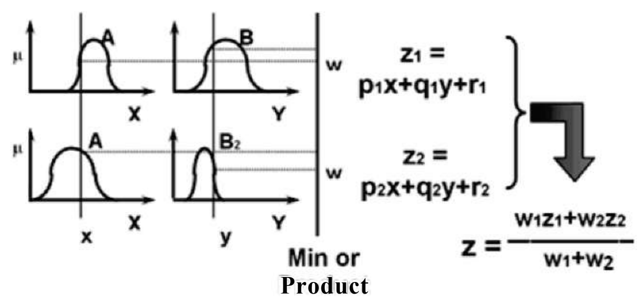

Fig. 1. A scheme of a Sugeno-type FIS.

ᶠTo whom correspondence should be addressed.
E-mail: morteza.mohammadzaheri@adelaide.edu.au

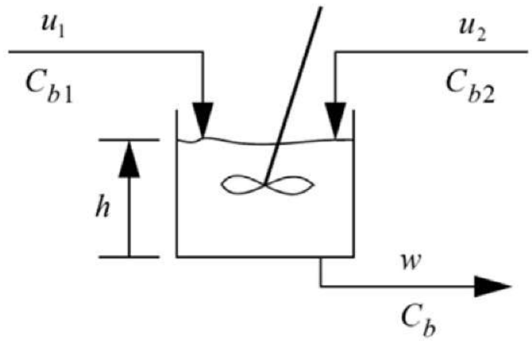

Fig. 2. A schematic of the studied CSTR [7].

first-order Sugeno-type FIS, the consequents of rules aie linear crisp functions of the inputs, independent of antecedent fuzzy values. For an FIS with M inputs:

$$z, = 2,ajXj+\&M+1. \quad j=1 \tag{2}$$

z,=output of i^{th} rule, x_j=j^{th} input.

The total output of a Sugeno-type FIS, N having rules, is calculated by using the following equation:

$$\text{output of FIS} = - \quad \sum_{i=1}^{N} \tag{3}$$

PROBLEM STATEMENT

The case study is a catalytic continuous stirred tank Reactor (CSTR). A diagram of the process is shown in the following figure:

Two flows of liquid enter the reactor with the concentration of C_M=24.9 (kmol/m^3) and C_{b2}=0.1 (kmol/m^3). The flow rates of high and low concentration input flows are named u_1 and u_2, respectively. The reactor outputs another flow of liquid with the concentration of C_b and the flow rate of w. Another important variable is the height. A simplified mathematical model of the system, achieved by mass balance equations, is:

$$ddt- = u1(t)+u*(t) - 0.2\text{^}(t), \tag{4}$$

$$\frac{dC_b(t)}{I} = [C_{b1} - C_b(t)] \frac{u\text{^}A}{ht)} + [C_{b2} - C_b(t)] \frac{U2^{(}t)}{hot)} - \frac{kiCbffl}{1+kA(t)\sim 2} \tag{5}$$

where the concentration of outlet flow and the height of liquid are considered as the outputs (w=0.2,/h).

The control of outlet concentration of the aforementioned system is addressed in this paper. This control problem is a successful case study for neural or neuro-fuzzy predictive control [7]. In neuro-predictive control, usually the low concentration flow (u_2) is set to a fixed value (e.g., 0.1 liters/s) and the control algorithm adjusts the other flow (u_1).

In spite of all the advantages of neuro-predictive control, formed by neural network models and derivative based control algorithms, it was observed that this method cannot be effectively used for double-command control of this system. In neuro-predictive control, using both flows does not lead to any improvement in the performance of the control system compared to a single-command one. Furthermore, in neuro-predictive control, an optimization problem should be solved to generate the control command. This process is highly time-consuming for double-command control, especially if the second order optimization algorithms, which are more reliable, are employed. In the next section, a brief explanation and the results for single command control of the studied CSTR system is presented.

SINGLE COMMAND NEURO-PREDICTIVE CONTROL OF CSTR (A BRIEF REVIEW)

In nonlinear predictive control, nonlinear models are used to predict the behavior of nonlinear systems, and an optimization method generates the control command based on minimizing a performance function involving predicted errors (such as following function):

$$J(k) = \sum_{i=1} [y,(k+i) - yd]^2 + p[u'(k) - u(k-1)]^2 \tag{6}$$

where y_s and y_d are the predicted and desired outputs of the system, respectively, and u' and u are tentative and actual control inputs. Additionally, p is a factor defining the importance of the constancy of control input.

Eq. (6) is a typical performance function (represented by J), which is usually used in neuro-predictive control. In discrete domain, at the instant of k, the output of the system is known (y(k)), and the tentative control command (u'(k)) is subject to optimization.

If current output and previous output/input of the system and u' are known, all other arguments of J will be definitely known. Fig. 3 shows how an estimated output is generated using tentative input and the current output of the system. However u' can be changed arbitrarily and freely from the recorded input/output data and this change affects other arguments of J, and, consequently, the performance function itself. Therefore, in the optimization for control purposes, it can be assumed that

$$J=J(u). \tag{7}$$

Finding u' so as to minimize the performance function is the final stage at nonlinear predictive control.

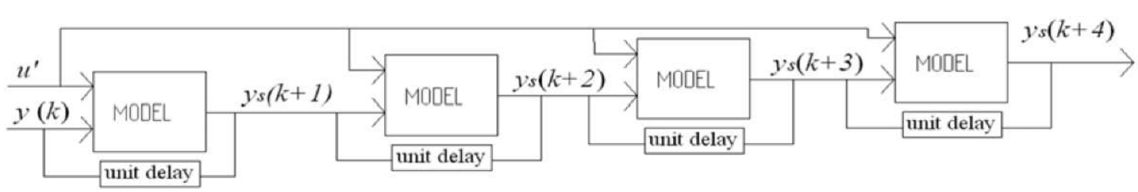

Fig. 3. Prediction of output values with the horizon of 4.

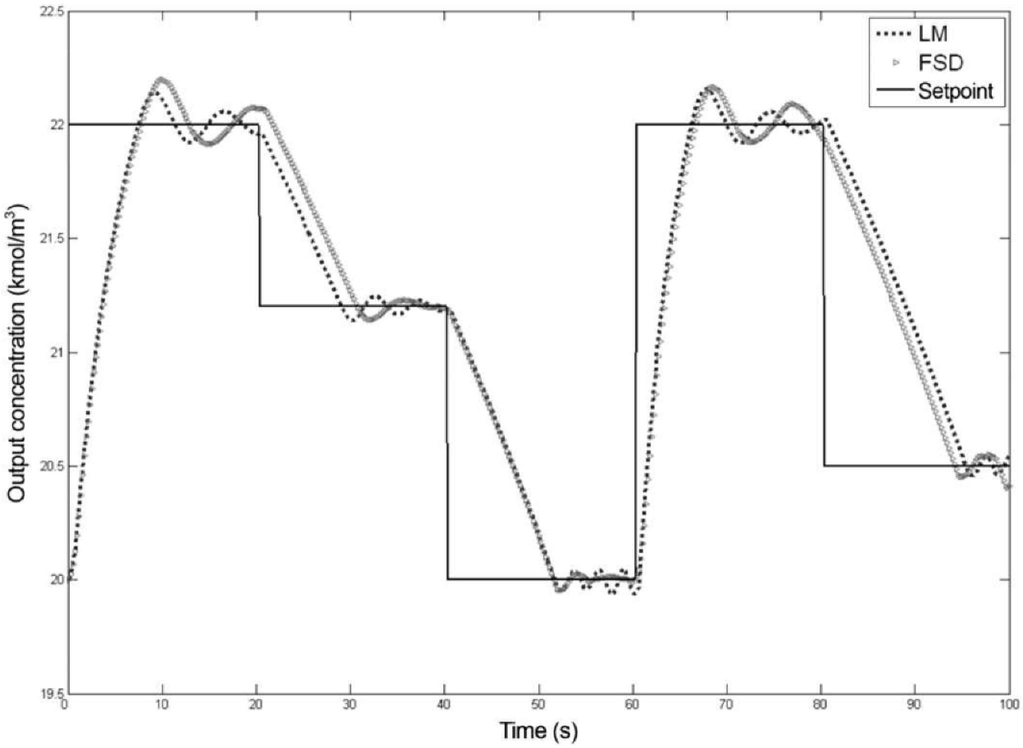

Fig. 4. Simulation results for different optimization methods.

Table 1. Simulation results for different optimization methods

Optimization method	EI ($kmol/m^3$)	IC (liters)	Simulation time (s)
LM	0.3651	0.0939	225
FSD	0.3729	0.0944	25
SD	0.7738	0.2553	24

Two design criteria are defined, being the error integral and the constancy of input (usually in the form of a flow rate):

EI = - fjeldt (8)

IC = - fWt+At) - u(t)| dt (9)

The results are shown in Table 1 and Fig. 4. The initial height of the tank is 30 cm and the initial value of outlet concentration of tank is 20 $kmol/m^3$. In Table 1, 'Simulation Time' is the time needed to simulate 100 seconds of operation of the closed loop system, with sampling time of 0.2 s, using a dual core processor (4,200 MHz) and MATLAB software. In this example, the reference changes very quickly to test the capabilities of the controllers. In optimization methods, "LM" stands for Levenberg Marquardt, "SD" stands for steepest descent and "FSD" stands for fuzzy steepest descent. More details about neuro-predictive control of CSTR are available in the appendices. Appendix A is about neural network modeling of the system (with one control command), and appendix B is about the utilized optimization algorithms.

DOUBLE COMMAND CONTROL OF CSTR

In this section the design of a control system to command both inlet flows (valves) is addressed. The control command is the sum of a transient control command, whose increments are adjusted by a fuzzy inference system, and a steady state control command. Transient control command pushes the system towards the desired situation, and steady state control command maintains the desired situation. At first, the fuzzy controller, generating the increments of transient control command, is designed; then the steady state control law will be introduced.

1. Fuzzy Controller/Transient Control Command

In this sub-section, initially the architecture of the transient control system is proposed; then the fuzzy rules forming the fuzzy logic controller are addressed. The absolute value of error (E) and its differential (dE) are the inputs to the fuzzy controller.

$$dE=E(1-z^{-1}) \tag{10}$$

where z^{-1} is unit delay.

The maximum output of the fuzzy controller is set to 0.1 due to practical limitations of the valves. If the error is positive, that is, the concentration is lower than its desirable value, the output of fuzzy controller is added to u1, otherwise it is added to u2. This decision is made by **f1** function shown in Fig. 5. After adding fuzzy controller output to the delayed control commands, both control commands pass through **f2** function. In **f2,** if the error is positive, u_2 is set to zero; otherwise u_1 is set to zero. Also, if E>2, non-zero control command is set to four. Saturation functions guarantee that the generated control command (transient control command) is in the range of [0 4], the acceptable range for the control valves.

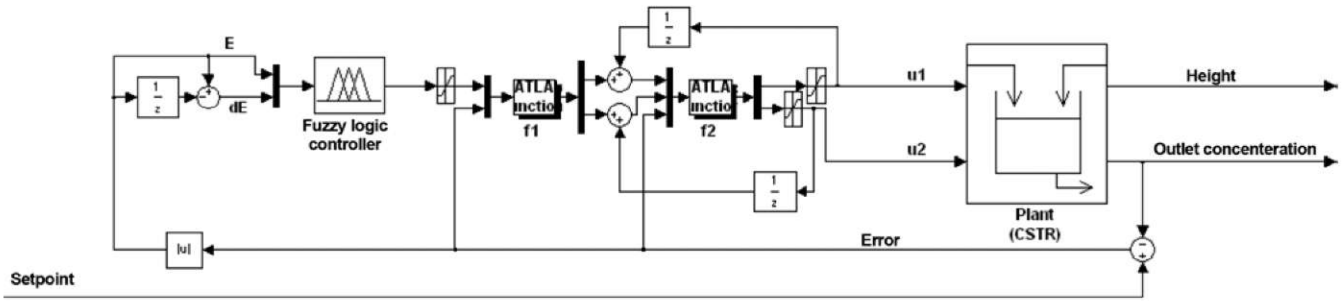

Fig. 5. Control circuit for transient mode of control.

Before addressing fuzzy rules, the membership functions of E and dE are introduced. In general, a membership function should have the following characteristics:

lim^rfu^E) = 0
E —be
lim^d™ (E) = 0
E— 0 (11)

lim,u%A(E) = 0
E- 0
lim fihigh(E) =1
E—be (12)

lim Hgood/bJk dE) = 0
dE—0
lim fisood(d dE) =1
dE—bde
lim HbaAdE) =1
dE—bde (13)

lim flzero(E) = 0
E—ce
lim^ze,o(E) =1 (14)

where, *be* stands for big absolute error (E), *ce* stands for considerable absolute error (E), and *bde* stands for big error differential (big dE).

These parameters are chosen by the designer based on knowledge about the system. The selected membership functions, in this article, are shown in Figs. 6 and 7.

Among E membership functions, "medium" is triangular, and "high" and "zero" are Gaussian:

MMA E) = exp (- 2(E-f)^3) (15)

Mzero(E) = exp (- 2V 0.0V) (16)

dE membership functions are shown in Fig. 7 and Eq. (17):

dE > 1 ^^bad(dE) =1
dE <-1 ^MgoU dE) =1 (17)

Membership function "zero" is only used in the damper rule which will be introduced later in this section. Other membership functions (two for E and two for dE) are used in the design at this stage. With two fuzzy values (membership functions) for any inputs to the fuzzy controller, four different compositions can be made for the antecedent part of fuzzy rules. These quadruple compositions need to be arranged in terms of the criticalness of the system situation. Table 2 presents such an order. For instance, the worst situation

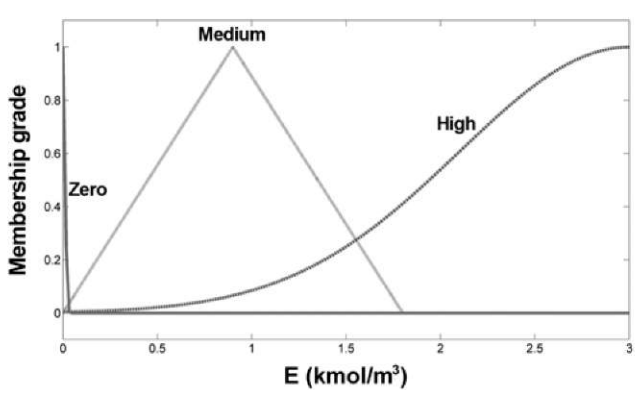

Fig. 6. Membership functions of E (absolute error).

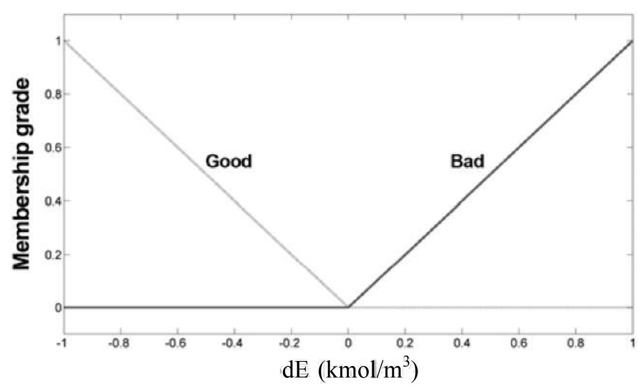

Fig. 7. Membership functions of dE.

Table 2. The order of possible situations of the system in terms of criticalness

	E	dE
1	medium	good
2	medium	bad
3	high	good
4	high	bad

occurs when E is high and dE is bad, which means E is increasing.

Four principal rules of the controller are defined based on the aforementioned situations of the system.

If the absolute error is high, the two following rules make the system decrease the error very quickly.

Rule 1: IF E is high AND dE is bad THEN du_I=0.1

Rule2: IF E is high AND dE is good THEN du_J=0.3E

If the error is not very high, the following rules will be activated to moderate the approaching speed towards the setpoint/reference and to avoid overshoot.

Rule3: IF E is medium and dE is bad THEN du_{JJJ}=0.2E

Rule4: IF E is medium and dE is good THEN du_{JF}=0.1E

Fig. 8 shows the control behavior of the system when a fuzzy controller containing the aforementioned fuzzy rules is applied.

With the same initial values as the plot shown in Fig. 4, the error integral and input constancy of the system (Eq. (8) and (9)), are IC= 0.0605 litres and EI=0.1772 kmol/m^3. The results are acceptable compared to single-command neuro-predictive control in terms of having reasonable values of IC and EI, which are important from the viewpoint of implementation and accuracy, respectively.

However, a chattering is observed when the system's output is close to the setpoint/reference. Fig. 9 shows control commands (inputs) versus time for the operation period, for which the response is shown in Fig. 8. It is observed that in time periods such as 50-60 s or 90-100 s, changes in control input occur which lead to chattering. Frequent opening and closing of the valve is problematic in practice.

In order to avoid chattering in the vicinity of the setpoint, a damper rule is added to the fuzzy controller:

Rule5: IF E is zero THEN du_r=0 (damper rule)

This rule improves both design criteria, IC=0.0383 litres, and EI=0.1700 kmol/m^3. Zero membership function is intentionally selected very narrow; a wider zero causes a considerable loss in error integral. The main role of the fifth rule is the diminution of frequent changes of control inputs, and its consequent chattering, when the system's output is in the vicinity of the setpoint.

2. Steady State Control

The designed fuzzy controller is an error-based controller; that is, the only entering signal to the controller is the error. Considering Fig. 8-11, it is observed that even when the error is zero, or very close to zero, the system's output and consequently the control input is subject to change (consider, for example time periods of25-40 s, 45-60 s or 85-100 s). In the designed fuzzy controller, if the error is zero, the transient control input is zero. The value of zero for the control input cannot maintain the desired situation (Figs. 8 and 10). As a result, a steady state control command is added to transient control command (generated by fuzzy controller); when the error is around zero, transient control command approaches zero and steady state control command maintains the desirable situation, that is, keeps the system's response fixed.

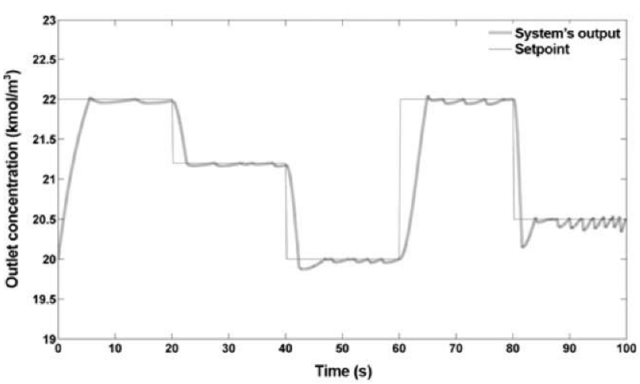

Fig. 8. The response of system with fuzzy control (without damper rule).

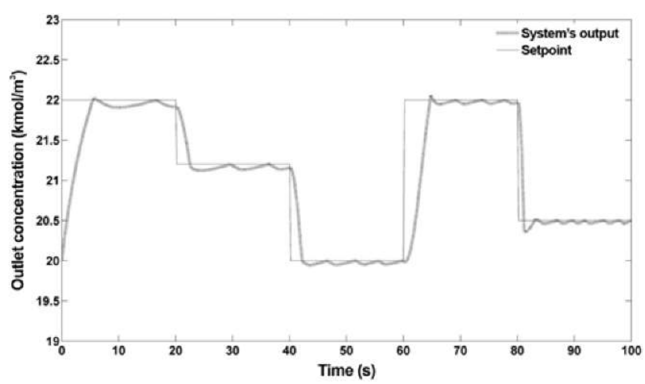

Fig. 10. The response of system with fuzzy control (with damper rule).

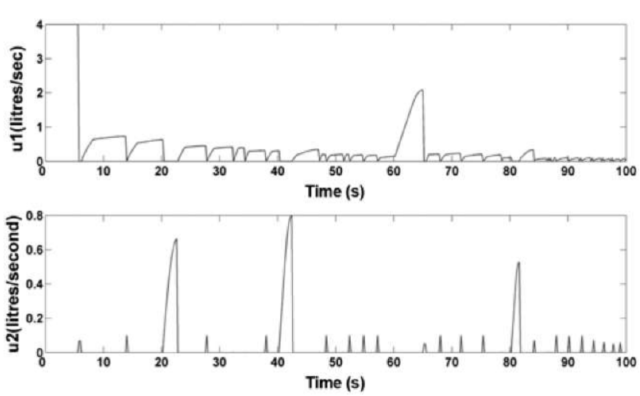

Fig. 9. Control commands generated by fuzzy control system of Fig. 5 (without damper rule).

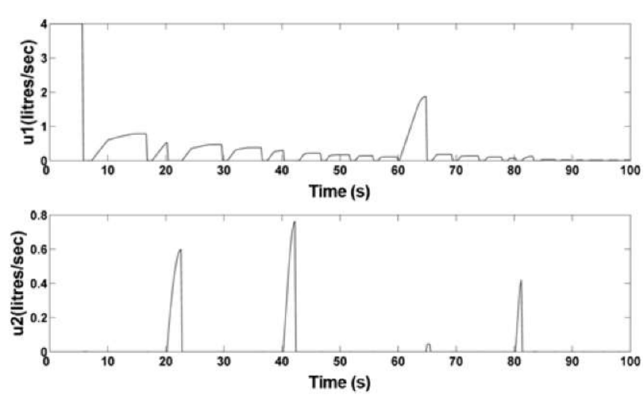

Fig. 11. Control commands generated by fuzzy control system of Fig. 5 (with damper rule).

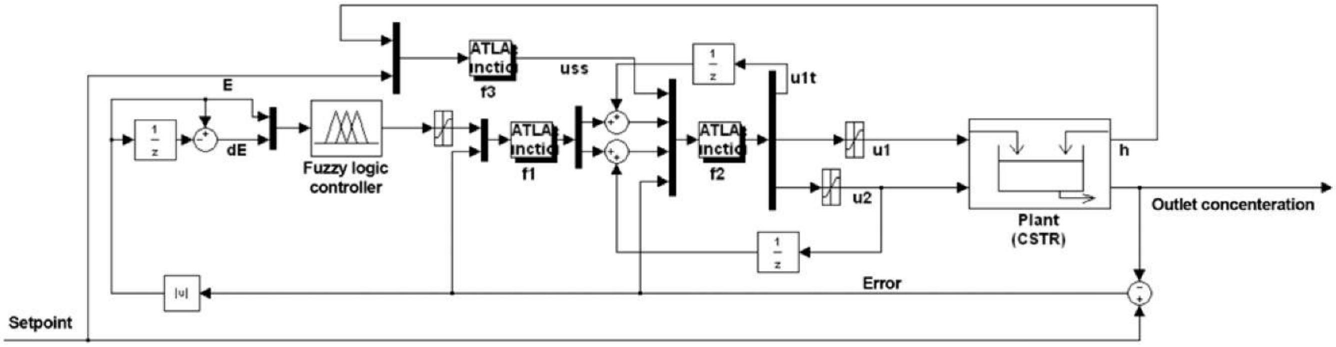

Fig. 12. Control circuit.

In total, at steady control situation:

$$
\begin{aligned}
&u_1 = \\
&u_2 = 0 \\
&\frac{dC_b(t)}{dt} = 0 \\
&C_b(t) = r(t)
\end{aligned}
\tag{18}
$$

where r(t)=reference.

In order to find steady state control command, the physics-based model offered in Eq. (5) is used:

$$\frac{dC_b(t)}{dt} = [C_{b1} - C_b(t)]\frac{u_1(t)}{h(t)} + [C_{b2} - C_b(t)]\frac{u_2(t)}{h(t)} - \frac{k_1 C_b(t)}{(1+k_2 C_b(t))^2} \tag{5}$$

Considering the aforementioned conditions, Eq. (5) changes to:

$$[24.9 - r(t)]\frac{u_1(t)}{h(t)} - \frac{k_1 C_b(t)}{(1+k_2 C_b(t))^2} = 0, \text{ or}$$

$$u_{1s}(t) = \frac{k_1 C_b(t)\, h(t)}{(1+k_2 C_b(t)^2)(24.9 - r(t))} \tag{19}$$

The obtained steady state control command, dependent on both level height and the reference (setpoint), is calculated in **f3** function (Fig. 12). Having steady state control command, the first valve is always open ($u_1>0$), so when error is negative (the outlet concentration is higher than its desirable value), the performance decreases and it takes longer for the system to overcome negative error, since a positive u_1 increases the concentration. In order to compensate for this drawback, **f2** function sets u, (the steady state control command) to zero as error<-0.5 kmol/m^3. Moreover, the final control command is generated in **f2** by adding two control commands.

Adding steady state control command improves input constancy significantly to IC=0.0305 liters, but the error integral increases to EI=0.1788 kmol/m^3. As the main advantage, the control input changes very smoothly, so this combined control command is more suitable for real application.

STABILITY REMARK

Stability discussion is done based on two practical assumptions, rather than mathematical model, which are evident for the case study and can be paraphrased for a wide class of systems. These assumptions are the basis of stability discussion.

$\forall (C_{b1} > C_b > C_{b2},$
A1: if (u_1=4 litres/min & $u_2 = 0$) $\rightarrow \dot{C} > 0 (e<0)$
A2: if (u_2=4 litres/min & $u_1 = 0$) $\rightarrow \dot{C} < 0 (e>0)$

In the first-order systems which control input affect the first derivative of the output (e.g. heat-related systems), there usually exists a value of control input that changes the sign of the first temporal derivative of the output immediately after application. As a result, two proposed assumptions can be restated for other similar systems.

To address bounded-input bounded-output (BIBO) stability, it is proved that if error square or the absolute value of the error, is higher than a bounded value, this value definitely decreases. So, the error, and the output, always remains bounded if it is bounded in the beginning. The decrease of error square means the derivative of error square is negative. Since$(d/dt)e^2=2e\dot{e}$ as the stability criterion, it is needed to prove if the absolute value of error (or error square) is higher than a bounded value then:

$$e\dot{e} < 0 \tag{20}$$

In this section, the value of 3 kmol/m^3 is considered as the boundary of absolute value of error, and it is proved that as the absolute value of error is higher than 3 kmol/m^3, error square decreases, and error will not be unbounded.

$$e > 3 \text{ kmol/m}^3 \xrightarrow{f2} (u_1=4 \;\&\; u_2=0) \xrightarrow{A1} \dot{e}<0 \rightarrow e\dot{e}<0,$$

$$e < -3 \text{ kmol/m}^3 \xrightarrow{f2} (u_1=0 \;\&\; u_2=4) \xrightarrow{A2} \dot{e}>0 \rightarrow e\dot{e}<0.$$

SUMMARY OF RESULTS

In this section, with a new set of setpoints/references and initial height (60 cm), all three control systems are checked again, including fuzzy controller system (FC), fuzzy control system with damper

Table 3. Simulation results for different control systems

	EI (kmol/m^3)	IC (litres)
FC	0.6088	0.0819
FCDR	0.6528	0.0743
Hybrid	0.6043	0.0556

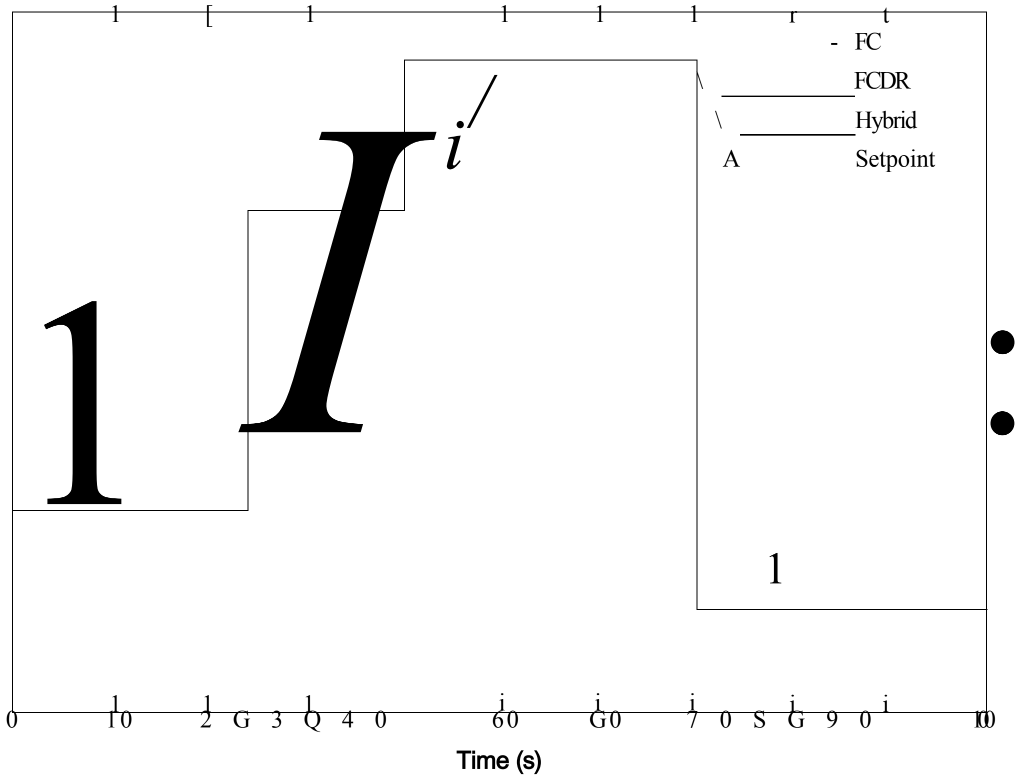

Fig. 13. The response of the system.

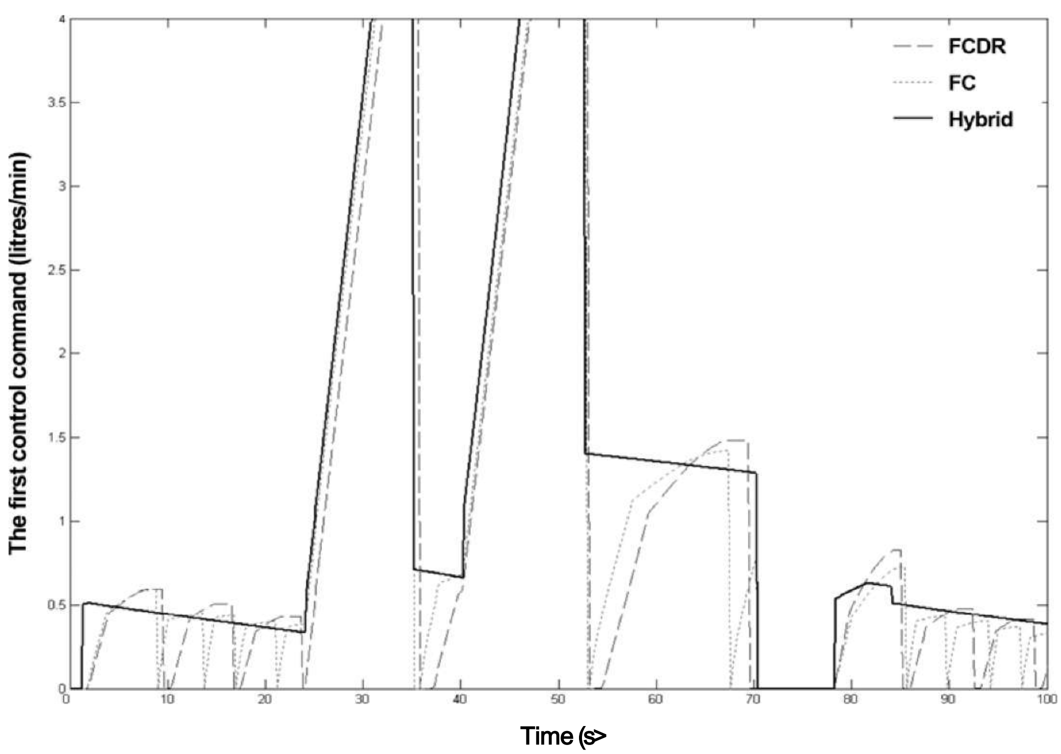

Fig. 14. The first control command during operation shown in Fig. 13.

rule (FCDR) and hybrid control system (Fig. 13, Table 3).

As it is indicated in Fig. 14, the change of control input in the proposed hybrid control system is very smooth. Also, in all the simulations shown in Fig. 13, the time needed for simulation is around 5 seconds (compare with Table 1). There are two more relevant plots in Appendix C.

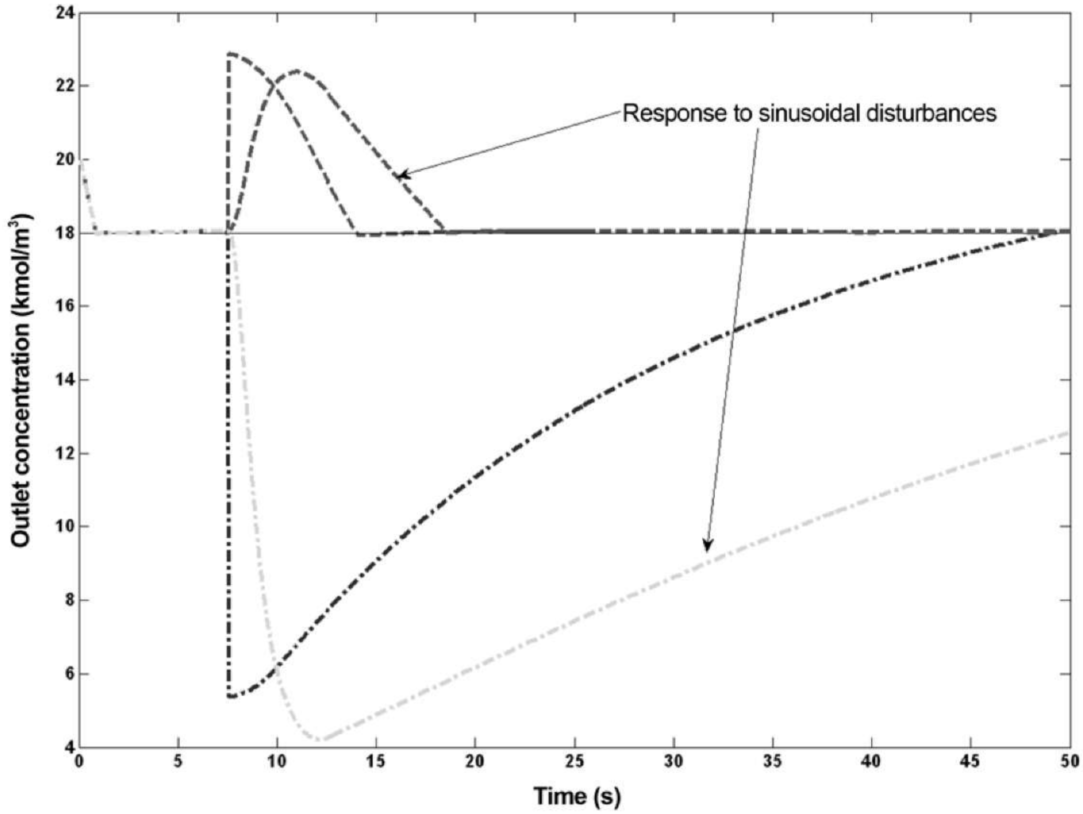

Fig. 15. The response of system to disturbances.

DISTURBANCE REJECTION

To check the capability of the hybrid control system in rejecting disturbances, four very severe disturbances were applied to the system. First, 4 liters of low or high concentration liquid was poured suddenly into the reactor (in 0.2 second). Both disturbances (high and low disturbances) were successfully rejected as shown in Fig. 15 (also, Fig. 19 in Appendix C offers some complementary information). Then 4 liters of low or high concentration liquid was poured to the system in 10 seconds as a sinusoidal disturbance function.

ROBUSTNESS AGAINST NOISES AND UNCERTAINTIES

The feedforward controller is the only model-based part of the proposed hybrid control system. Feedforward controllers are usually more sensitive to noise and parameter uncertainties. High sensitivity to uncertainties or noises, due to model-based feedforward controller, could be a serious defect of the proposed control system. To address the aforementioned issue, the feedforward control command was multiplied by a 'Test Coefficient' before being added to feedback (transient) control command. This means that feedforward control command would no longer remain as accurate (this inaccuracy can be caused by noise or uncertainty, in reality). The effect of this situation on the control system was then checked. Table 4 shows the values of design criteria for different values of 'Test Coefficient' (see Eq. (8) and (9), and Table 3). Even a considerable inaccuracy (50%) does not deteriorate control behavior significantly.

Table 4. Simulation results for hybrid system at different test coefficients

Test coefficient	EI (kmol/m^3)	IC (liters)
0.5	0.6081	0.0608
0.7	0.6090	0.0569
1	0.6043	0.0556
1.3	0.6523	0.0573
1.5	0.6761	0.0609

Error integral remains reasonably small. Furthermore, the value of input change remains low, as a crucially important advantage in terms of implementation, at all values of test coefficient shown in Table 4.

CONCLUSION

After disappointing results of using neuro-predictive technique in double command control of the outlet concentration of a nonlinear CSTR, a hybrid control system was designed in this research to adjust simultaneously both entering flows of a nonlinear CSTR. The proposed hybrid includes a model-free error-based fuzzy controller and a model-based, but very robust against model uncertainties, non-error-based steady state control law, The fuzzy controller pushes the system towards the reference. A fuzzy rule (damper rule) is deliberately added to the fuzzy controller to reduce the control input's frequent change and consequent output's chattering. Steady state control maintains a desirable situation. The input to steady state control law is the reference (setpoint) and measurable states of the system which are not subject to control (height, in this case study). The performance, efficiency and input constancy, achieved by the proposed hybrid control system, are significantly higher than those of single-command neuro-predictive controllers which have already been designed by the authors and known as a successful method in this case study. The proposed method particularly suits real application in terms of trifling computations and control input change. Furthermore, it is proved that the proposed control system is BIBO stable.

NOMENCLATURE

a : parameters of consequent part of fuzzy rules
A : assumption
BIBO: bounded input-bounded output
C_b : outlet concentration of CSTR [kmol/m^3]
C_M : the concentration of the first inlet flow to CSTR [kmol/m^3]
C_{b2} : the concentration of the second inlet flow to CSTR [kmol/m^3]
CSTR : catalytic stirred tank reactor
d u ^ : consequents of fuzzy controller rules [litres/min]
e : error [kmol/m^3]
E : absolute value of error [kmol/m^3]
EI : error Integral [kmol/m^3]
F, **f** : function
FC : with fuzzy controller
FCDR : with fuzzy controller having damper rule
FSD : (with) fuzzy steepest descent method
g : defined in (34)
G : defined in (35)
h : level height (cm)
IC : input constancy criterion [litres]
J : performance function
Kj_2 : CSTR parameters relevant to resistance of valves
LM : (with) Levenberg-Marquardt method
PAN : prediction accuracy for N next instants [kmol/m^3]
r : reference [kmol/m^3]
SD : (with) Steepest Descent
t : time [s]
Time : time needed for the simulation of control system for 100 seconds [s]
u : control input [litres/min]
u' : tentative control input [litres/min]
u_1 : volume rate of high concentration input to CSTR [litres/min]
u_2 : volume rate of low concentration input to CSTR [litres/min]
w : weight of a fuzzy rule
x : input to a fuzzy rule
y : output of the system
z : output of a fuzzy rule
z^{-1} :unit delay function [1/s]
p : a factor defining the importance of the constancy of control input
H : membership grade
T : time period of operation (s)

Superscript
^ : estimated

Subscripts
d : desired
k : numerator
s : predicted
ss : steady state
tr : transient

REFERENCES

1. D. L. Yu, T. K. Chang and D. W Yu, *Control Engineering Practice,* **15,** 1577 (2007).
2. C. R Madhuranthakam, A. Elkamel and H. Budman, *Chem. Eng. Process.,* **47,** 251 (2008).
3. L. Feng, J. L. Wang and E. K. Poh, *Journal of Process Control,* **17,** 683 (2007).
4. W. Wu, *Journal of Process Control,* **13,** 525 (2003).
5. J. Prakash and R. Senthil, *Journal of Process Control,* **18,** 504 (2008).
6. R. K. Al Seyab and Y Cao, *Comput. Chem. Eng.,* **32,** 1533 (2008).
7. H. Demuth, M. Beale and M. Hagan, *Neural networks toolbox 5, user 's guide,* The MathWorks, Online (2007).
8. Y Cao and P. M. Frank, *IEEE Transactions on Fuzzy Systems,* **8**(2), 200 (2000).
9. Y Oysal, Y Becerikli and A. F. Konar, *Comput. Chem. Eng.,* **30,** 878 (2006).
10. K. Belarbi, F. Titel, W. Bourebia and K. Benmahammed, *Engineering Applications of Artificial Intelligence,* **18,** 875 (2005).
11. C. Karakuzu, *ISA Transactions,* **47,** 229 (2008).
12. B. Ding and B. Huang, *International Journal of Systems Science,* **39,** 487 (2008).
13. W Hwang, J. Chey and H. Rhee, *Journal of Applied Polymer Science,* **67,** 921 (1998).
14. P. Christofides and P. Daoutidis, *Automatica,* **32**(H), 1553 (1996).
15. M. Mohammadzaheri and L. Chen, *Efficient intelligent nonlinear predictive control of a chemical plant,* 15th International Conference on Neural Information Processing of the Asia-Pacific Neural Network Assembly, November 25-28, Auckland, New Zealand (2008).
16. Y. Tan and A. R. Van Cauwenberghe, *Neurocomputing,* **10,** 83 (1996).
17. J. R. Jang, C. Sun and E. Mizutani, *Neuro-fuzzy and soft computing,* Prentice-Hall of India, New Delhi (2006).
18. J. Dennis and R. Schnabel, *Handbooks in operations research and management science,* Vol. **1,** Optimization, Chapter I A view of unconstrained optimization, 1 (1989).

APPENDIX A: NEURAL MODELING OF CSTR (WITH SOLE CONTROL COMMAND OF u_1)

The modeling was performed particularly for the purpose of predictive control. The studied CSTR has two control inputs, u1 and u2. One control command is used in predictive control, so the flow rate of the second input flow (with the concentration of 0.1 kmol/m^3) is set to the constant value of 0.1 liters/s. As a result, this value is not considered in modeling as an input signal anymore. Moreover, the order of two is assumed for the model. This model (presented in Eq. (21)) is used to find the first estimated value of C_b:

$$[C_b(k+1), h(k+1)] = F[u1(k-1), u1(k), Cb(k-1), Cb(k), h(k-1), h(k)] \quad (21)$$

or

$$C_b(k+1) = F1[u1(k-1), u1(k), Cb(k-1), Cb(k), h(k-1), h(k)] \quad (22)$$

$$h(k+1) = F2[u1(k-1), u1(k), Cb(k-1), Cb(k), h(k-1), h(k)] \quad (23)$$

After very first instants of the prediction:

$$[C_b(k+1), II(k+1)] = F[u1(k-1), u1(k), C_b(k-1), C_b(k), h(k-1), h(k)] \quad (24)$$

or

$$C_b(k+1) = F1[u1(k-1), u1(k), C_b(k-1), C_b(k), h(k-1), li(k)] \quad (25)$$

$$h(k+1) = F2[u1(k-1), u1(k), C_b(k-1), C_b(k), h(k-1), h(k)] \quad (26)$$

where variables with a hat are the estimated ones.

Although often only one predicted value is used in predictive control (i.e. C*b),* all the outputs should be estimated, because most of systems are dynamic and the outputs are usually coupled (in this problem, h, as the representative of liquid volume, affects the value of C_b). Therefore, the estimated values of all the outputs are needed to predict any of them, for a period of time in the future.

After the definition of the model's order, the training data should be normalized and arranged. 8,000 set of data (including u_1, h and C*b)* with the sampling time of 0.2 second are utilized in training. The normalized data are arranged as below:

Inpu'

u1(1)	u*(2)	Cb(1)	Cb(2)	h(1)	h(2)
$u_1(7998)$	$u_1(7999)$	$C_b(7998)$	$C_b(7999)$	h(7998)	h(7999)

Output

Cb(3)	h(3)
Cb(8000)	h(8000)

(27)

A four-layer recurrent perceptron is trained by using the prepared data (Eq. (27)). The input layer of the utilized perceptron has six neurons (equal to input signals). This ANN has one nonlinear (with sigmoid activation functions) and one linear (with linear activation functions with slope of 1) hidden layers. Both hidden layers have 13 neurons. The output layer also has two neurons with linear activation functions with a slope of 1. A linear hidden layer may seem useless at first glance, because a linear combination of the outputs of nonlinear hidden layer neurons is generated at the output layer, even without this linear hidden layer. In other words, the structure of mathematical relation between input and output of ANN is the same with or without the linear hidden layer, however, adding a linear hidden layer improves the accuracy, in practice. It seems a wider variety of adjusting parameters let the model be trained more successfully. The training method is the Levenberg-Marquardt error back propagation. The (batch) training has been performed in 100 epochs and the performance function is sum of squared errors (MSE).

In this research, two different series of checking data were used.

Table 5. Prediction accuracy for different trained models

Criterion	PA10 (kmol/m^3)		PA30 (kmol/m^3)	
Checking data	1$^{s'}$ series	2nd series	1$^{s'}$ series	2nd series
Complete perceptron (double output)	0.018	0.022	0.051	0.033

Both series are entirely different from training data.

A criterion is defined for the predictive accuracy of models, namely PAN:

$$PAN = 21C\,b(i) - Cb(i)| \quad (28)$$

Table 5 shows PA10 and PA30 (the sum of absolute error of prediction for 10 and 30 future instants or next 2 or 6 seconds), for two different series of checking data.

APPENDIX B: OPTIMIZATION

From section IV, it is found that for nonlinear predictive control purposes:

$$J=J(u). \quad (7)$$

Now, u' should be so determined that J has its minimal value. To do so, Taylor's series is written for performance function up to the first and second order:

$$J(u'+Au')=J(u) + Ju^{)}(Au'), \quad (29)$$

$$J(u'+Au-)=J(u) + J\,u\,W') + {}^{1}\text{-}^{\wedge\wedge}l|lU^{:\}}(Au')^2 \quad (30)$$

Based on these expansions, two different methods are used for optimization in this paper: Levenberg-Marquardt method, based on Eq. (30), which is a very good derivative based optimization method [16,17], it is currently used for neuro-predictive control [7]. The second method, based on Eq. (29), is a combination of steepest descent and fuzzy logic.

1. Levenberg-Marquardt (LM)

In this method, after derivation, Eq. (31) will be obtained:

$$\frac{9J(u'+AuQ}{9(Au)},, \frac{JO}{3u'} + \frac{9^2J(u')}{9u'^2}{}^{1}\,). \quad (31)$$

In order to minimize J(u'+Au), its derivative is set equal to zero. Consequently,

$$Au' = -\frac{-a^2J(u')}{9u'^2}\text{-}\;\frac{"JV}{3u'}. \quad (32)$$

The right-hand side of Eq. (32) is called Newton's direction [17]

Since Eq. (32) is an approximate relation, in order to guarantee that the performance function decreases at any stage, Eq. (32) is written in the form of Eq. (33):

$$Au' = -\frac{a^2J(u')}{9u'^2} + 1 \quad \frac{^\wedge Ju)}{9u'}. \quad (33)$$

In practice, the following relation is used:

A u ' = u'new - uOld = - (a^u1} / 9u'2 + 1 u . (34)

where; X = d x u—2 . (35)

An initial value is assigned to d (e.g. 0.001), then Sis generated:

S 9J(u1 / (d + 1)3 J - du' (36)

Then: if E(u'+^)<E(u') then d=d/10; otherwise d=dx 10; (37)
(10 is a modification factor, it can be of another value)

As the value of d is repeated, the algorithm stops.

Eq. (34) represents the Levenberg-Marquardt method for the optimization of a single variable function [17]. In this method, g is numerically considered as performance function gradient:

J u ') = / 9u' Bk J(k) - J(k-1) / u'(k) - u(k-1)' (38)

moreover, G_t is defined as:

J u T -1 / L 9u'2 . =G t u'(k)-u(k-1) / (gt - gt-1) (39)

So Eq. (34) can be rewritten in this form:

Au'=un,,-uOd=ˉ n(1+d)Gigi. (40)

Using Eq. (40), we will have:

J(un$_e$w)=J(u0id-n(1+d)$G_i g_i$), (41)

or: Argument of J=uOd- ((1+d)Gtgt. (42)

Both *U'M* and (1+d)$G_t g_t$ are known in this stage; then, with changing argument of J moves along a line. There is an optimum point on this line that minimizes J. Such an optimization problem is classified as a linear search. Backtracking method, introduced by Dennis and Schnabel [18], is selected for linear search. The modified u' (u'$_{new}$) is used as a new control input.

2. Fuzzy Steepest Descent (FSD)

A fuzzy-derivative optimization method is specially designed to suit optimization tasks for predictive control purposes.

In Eq. (29), if Au' is replaced by - (^ J p ^ then J(u'+Au')

• J < u ' > - J) ' (43)

If n>0, it can be concluded (approximately) J(u+A u)<J(u), (44)

Any positive value can be used for (For nonlinear predictive purposes, (can be generated by a fuzzy inference system (FIS) to reduce the alteration of the control system's response when it is approaching the setpoint/reference. This FIS has two rules:

Rule 1: if |e| is low then (=0
Rule 2: if |e| is high then (=1

Fig. 16 shows the membership function of high and low.

The designed FIS can be simplified to a simple function of |e|.

M'HIGH |e| (45)

For |e|<0.5: MW=-2|e|+1, (46)

Acoadmgt° q. (3) , (= [0x(-2|e|+1)] + [1x|e|] / +1)+N = ^e (47)

For |e|>0.5: MW=0 (48)

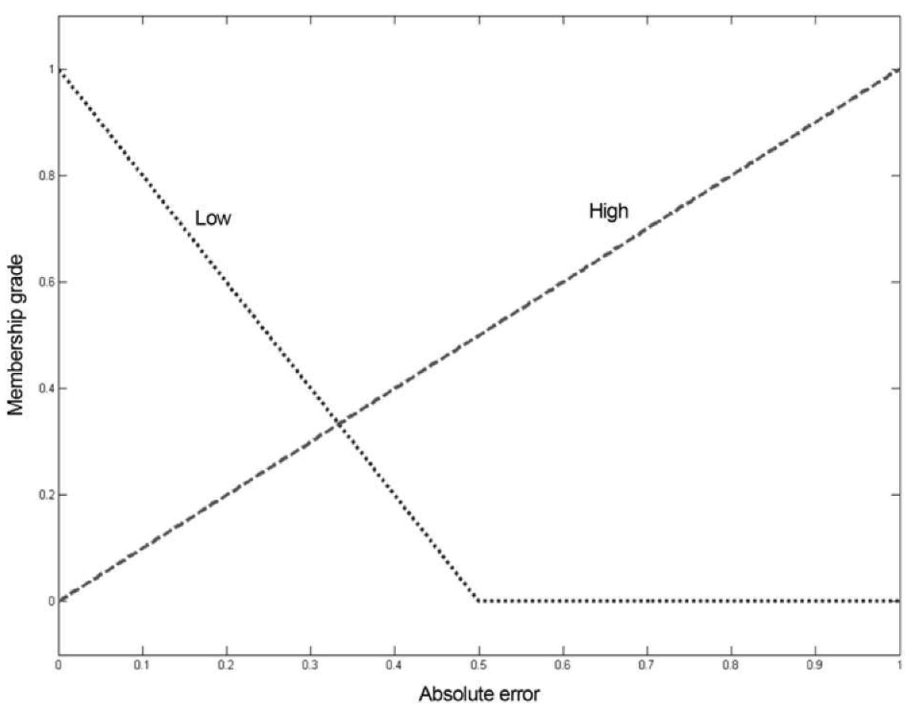

Fig. 16. Membership functions of high and low fuzzy values in fuzzy steepest descent optimization method.

According to Eq. (3), n [0X0M1XH] =1 (49)

In summary:

|e| < 0.5 ^

(50)

|e| > 0.5

For nonlinear predictive control purposes, the proposed fuzzy steepest descent method leads to much better control performance in comparison with classical steepest descent methods. In terms of control performance, fuzzy steepest descent is comparable with Levenberg-Marquardt method with around ten times less computation (Mohammadzaheri and Chen, 2008).

APPENDIX C: COMPLEMENTARY PLOTS

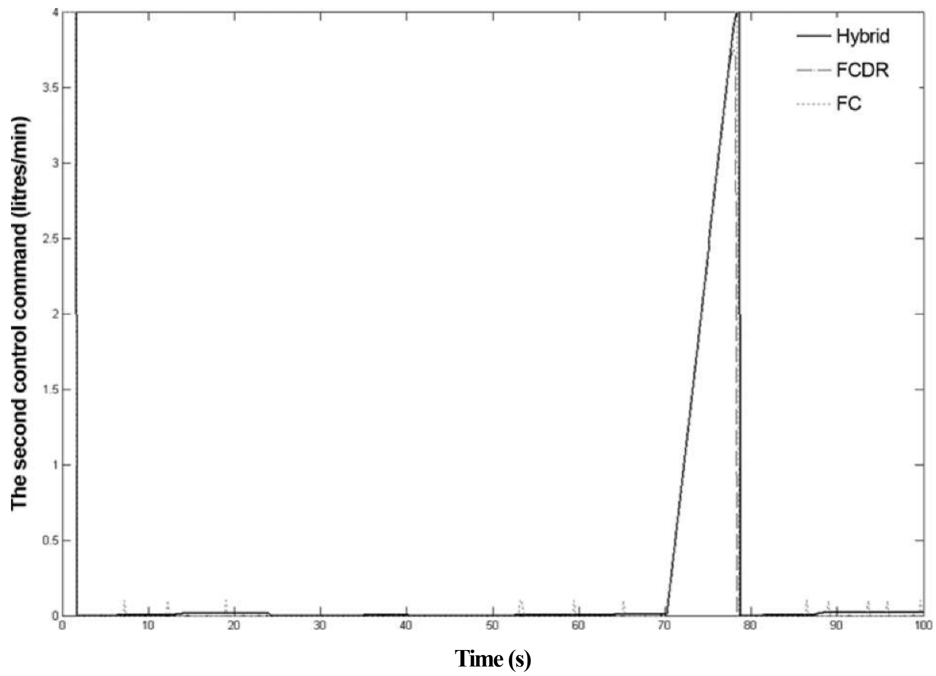

Fig. 17. The second output versus time, for the operation shown in Fig. 13.

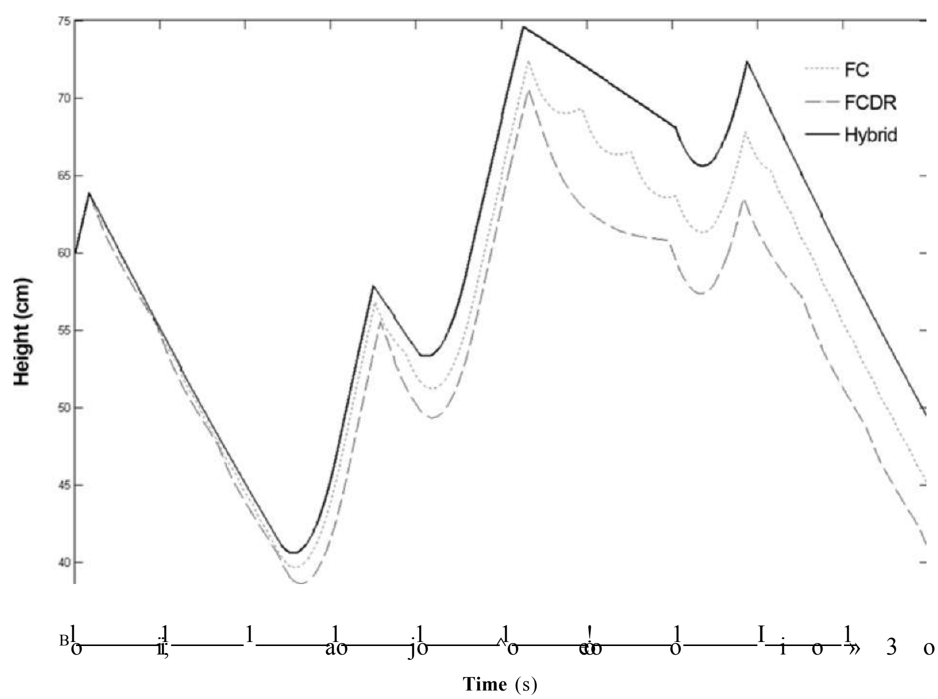

Fig. 18. The level height versus time, for the operation shown in Fig. 13.

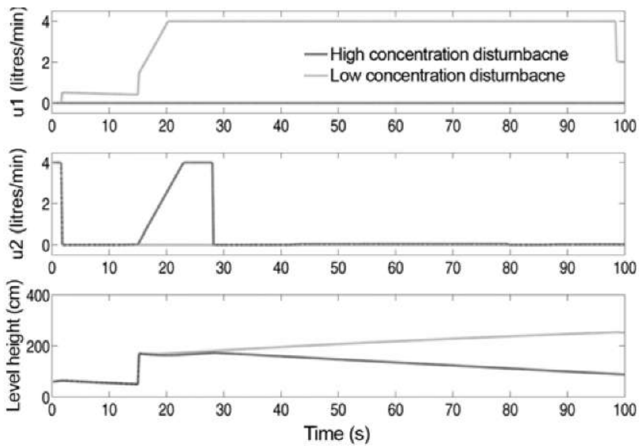

Fig. 19. Level height and control inputs during operation shown in Fig. 15 (instantaneous disturbances).