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AN OPTIMUM SOLUTION FOR A PROCESS CONTROL PROBLEM (CONTINUOUS STIRRED TANK REACTOR) USING A HYBRID NEURAL NETWORK.

[a] Emuoyibofarhe O.Justice, [b]Reju A Sunday

[a] Department of Computer Science and Engineering,
Ladoke Akintola University of Technology, Ogbomoso, Nigeria
[b] Department of Computer Sc. and Information Tech. National Open University of Nigeria
eojustice@justice.com, sunnyareju@gmail.com

All correspondence to: eojustice@justice.com or eojustice@gmail.com

ABSTRACT

Chemical process control requires intelligent monitoring due to the dynamic nature of the chemical reactions and the non-linear functional relationship between the input and output variables involved. CSTR is one of the major processing unit in many chemical, pharmaceutical and petroleum industries as well as in environmental and waste management engineering. In spite of continuing advances in optimal solution techniques for optimization and control problems, many of such problems remain too complex to be solved by the known techniques. Thus, a heuristic approach is often a viable alternative. Neural Network models offer the most unified approach to building truly intelligent systems, which can provide good optimal solution for many applications. In this work we propose a hybrid (KohKal) neural network algorithm which is being used to model and solve a continuous stirred tank mixer/reactor (CSTM/R) problem which is non-linear and stochastic in nature. This hybrid algorithm is robust and converges fast without been trapped into a local minimal, as is the case with the popular back-propagation neural network. We also establish the characteristic equations governing the dynamics of the Continuous Stirred Tank Mixer/Reactor. A controller model was formulated and tested and found to be consistently stable at varying conditions. The volume of the mixture in the tank was maintained as require to give enough hold up time to allow for adequate mixture of the contents in spite of the variations in the inlet streams. The calculated results agreed with the output of our neural network.

Keywords: *ANN, Kalkoh Hybrid Network, CSTR, Process Control Problem*

1. INTRODUCTION

Neural networks are well known for their ability to imitate the skill of experts by capturing knowledge, generalizing non-linear functional relationship between input- output variable, and they provides a flexible way of handling complex and intelligent information processing. Artificial Neural Networks (ANNs) have been shown to be effective as computational processors for various tasks including data compression, classification, combinatorial optimization problem solving, modeling and forecasting, adaptive control, multi-sensor data fusion, pattern recognition etc.

Control and optimization problems are some of the more difficult applications for ANN to master (Patterson, 1996). The mapping functions that must be learned are generally very complex in nature and the problem constraints that must be satisfied are often conflicting (Control problems typically require nonlinear time dependent mapping of input signals).

In process control, the ultimate goal usually is to detect or recognize abnormal process behavioral patterns and to find their corresponding causes or equipment / sensor whose malfunctioning have resulted to those faults. The faults usually present themselves in the following symptoms: deviation in flow, temperature and pressure leaks, blockage corrosion, wear, tear or mass transfer etc. (Watanabe et al. 1994, Himmelblau 1978). Most chemical process control occurs in a chemical plant (reactors, heat exchangers, pumps, distillation columns, absorbers, evaporators, tanks e.t.c). Chemical reactors are often the most difficult units to control in a chemical plant, particularly if the reactions are rapid and exothermic.

In this paper we proposed Kohkal network, which is a hybrid of the Counter-Propagation Neural Network (Kohonen Layer) and the Kalman Filter, which was used to model the dynamics of the CSTR problem and a typical problem was solved.

2. A REVIEW RELATED WORKS

Neural Networks based on adaptive resonance theory are equipped with unique computational abilities that are needed to function autonomously in a changing environment [Carpenter and Grossberg, (1988)], [Carpenter et al., (1992)] [Aldrich C., Moolman D.N and Van Deventer, (1995)] at the Department of Chemical Engineering at the University of Stellenbosch implemented a self-organizing and adaptive neural network system in the monitoring and control of the behaviour of an industrial/platinum flotation plant (Hydrometallurgical process). Other network formalisms; namely radial basis function (RBF) and adaptive resonance theory-2 (ART2) networks have also been employed for fault detection, diagnosis and process monitoring task [Leonard and Kramer, (1991)], [Whitley and Davis, (1994)]. Krishnaveni and Tulasi (2007) used ANN based systems to control patterns estimation for UPFC in power flow problem. [Zhang and Julian, (1994)] used a locally recurrent Neural Network to model the pH dynamics in a continuous stirred tank reactor (CSTR). Petia and Sebastiao (2006) applied a feed forward network in the modeling and control of a fed-batch crystallization process.

2.1 The Kohonen-Kalman (Kohkal) Algorithm

It is true that the Back Propagation Neural Network possess excellent pattern recognition, interpolation and generalization abilities, it is however faced with difficulties such as entrapment into a local minima during network training, long training times, and several runs are necessary to optimize networks. Hence we propose the Kohkal network, which is a hybrid of the Counter-Propagation Neural Network (Kohonen Layer) and the Kalman Filter. These networks have not been combined this way to the best of our knowledge in literature prior to or during this research.

The justifications for our hybrid network are the fact that

(i) it is believed that neural networks implementing both supervised and unsupervised learning algorithms are usually better than networks using only one learning algorithm.

(ii) The outputs of our Kohonen layer (which implements unsupervised learning) are entered as inputs into the Kalman's layer which uses a better iterative procedure to solve the linear system of equations.

2.2 DESCRIPTION OF THE KOHKAL NEURAL NETWORK

This Kohkal Network is prototype of the Counter Propagation Networks invented by Hecht- Nielson (1987). Kohkal shares a lot of similarities with the CPNN, except that the Grossberg's layer of CPNN implements Widrow-Hoff (Widrow-Hoff, 1960) rule while the Kalman layer of this Kohkal network uses an iterative procedure in handling the inputs.

The CPNN architecture is a combination of two well-known algorithms; the self-organizing map of [Kohonen, (1984)] and the Grossberg's out star [Grossberg, (1968)]. The CPNN has some advantages like the training algorithm is simple and fast [Peterson, (1992), Sorsa and Koivo, (1991)] and also that the optimal network architecture can be determined beforehand. Moreover, CPNN is not faced with entrapment into local minima problem. The Kohkal architecture (Fig.1) consists of three layers of neurons namely; Input, Kohonen and Kalman layers.

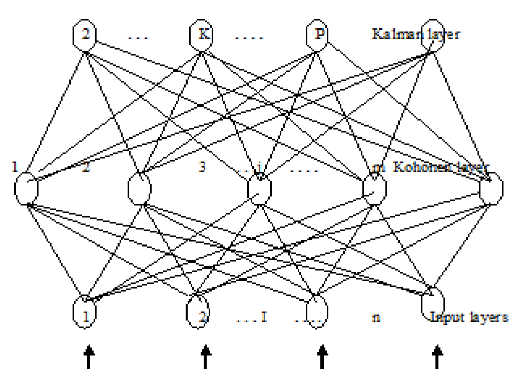


Figure 1 *Schematic architecture of the Kohkal Network*

FLOWCHART OF THE TRAINING ALGORITHM OF THE KOHKAL NETWORK

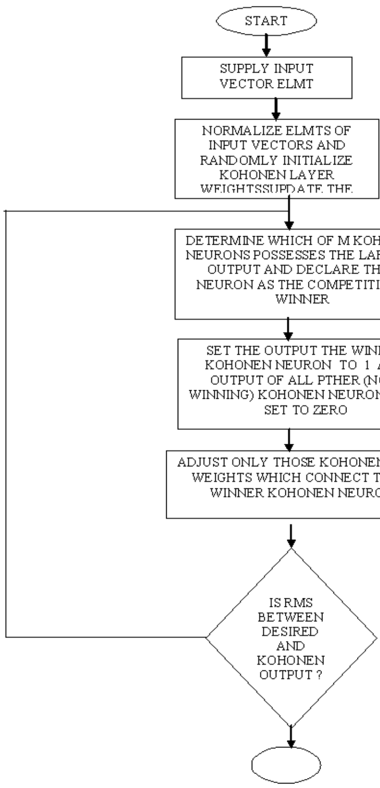
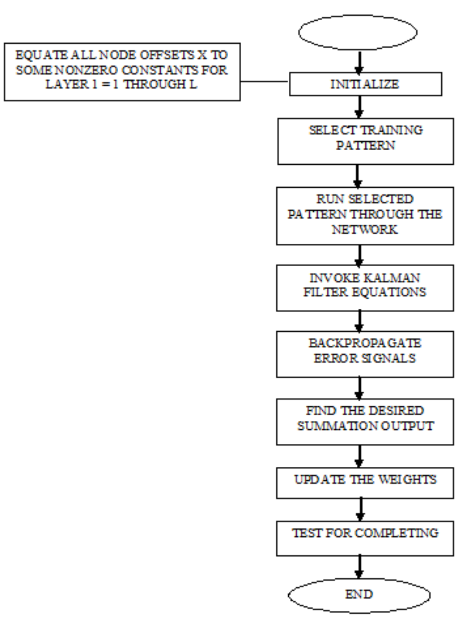


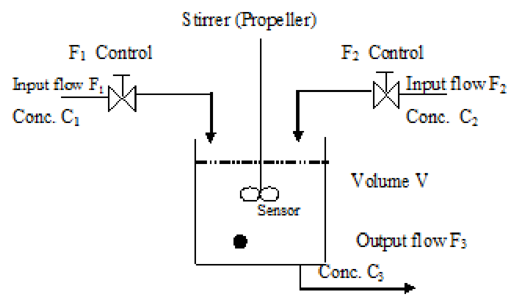
Figure 2. *A flowchart of the training algorithm of Kalkoh Network*



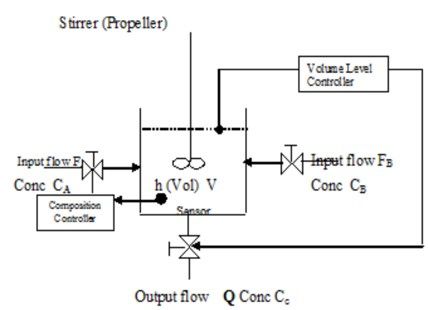
3. THE PROBLEM

The problem under consideration is a non-linear, stochastic problem which has practical application in many chemical, pharmaceutical and petroleum industries as well as in environmental engineering and waste management.

The problem is illustrated in fig.3(a) and (b) There are two input flows (with flow rates F1 and F2 , and concentrations C1and C2 respectively) going in at the top of the mixer/reactor. The two inputs are mixed in the tank to produce output with flow rate F3 and concentration C3 out at the bottom.



(a)



(b)

Figure. 3(a),(b) *A Continuous Stirred Tank Mixer (CSTM) / Feedback loop of the Continuous Stirred Tank Reactor (CSTR)*

The content of the tank is stirred continuously and hold time in the tank is assumed long enough to produce the desired degree of mixing. Input valves, and the output control the input flow rates F1 and F2 by a constant size orifice. The output flow rate is assumed to vary as the square-root of the static pressure head at the orifice. This means

$$F_3 = k\sqrt{V} \quad (1)$$

where V is volume of the material in the tank and K is an experimentally determined constant.
K = 0.02m 2/3 Sec.

The problem here is to control input flows F1 and F2 so that the output concentration C3 is as near as possible to a desired nominal (set) value C3o. At the same time, the volume of the mixture in the tank (V) is to be maintained at or near a desired nominal value so as to ensure both a sufficient and near constant output flow

i. The system under consideration is isothermal (i.e temperature is constant, and hence have no effect on the rate of reaction).
ii. Q is taken to be Turbulent condition of flow.
iii. Time of measurement of controllers, valves, measuring devices are assumed negligible. (Electronic Controller)
iv. Inlet composition of the streams does not change.
v. The disturbance is assumed to be from the flow-in alone.
vi. The rate of reaction r = kCACB or 2CACB
Where k = 2
vii. The set points are taken to be the steady state condition.

4. DYNAMICS OF THE PROBLEM

Recall the total material balance equation.

$$\frac{d(n_A)}{dt} = \frac{d(c_A V)}{dt} = \sum_{i:inlet} c_{Ai}F_i - \sum_{j:outlet} c_{Aj}F_j \pm rV \quad (3)$$

writing this in terms of the variables in figure 3.10, we have

$$\frac{dv}{dt} = \text{FA} + \text{FB} - \text{Q}. \quad (4)$$

(Assume at time t = 0, h = $\bar{h}$, FA = $\bar{F}$ A , FB = $\bar{F}$ B)
that is taking steady state condition as stated initially.

$$A\frac{\partial h}{\partial t} = \text{FA} + \text{FB} - \text{C}\sqrt{h}.$$

(5)

Linearizing gives:

The reaction between A and B follows a second order chemical reaction as stated below.

$$\text{A} + \text{B} \longrightarrow \text{C}, \quad \text{rA} = 2\text{CACB} \quad (2)$$

Also, it is desired that the mixture in the tank be maintained at a constant level or height h.[i.e controlling the volume]

Assumptions:

$$A\frac{\partial h}{\partial t} = \text{FA} + \text{FB} - [(\bar{c}\sqrt{\bar{h}} + \frac{\bar{c}}{2\sqrt{\bar{h}}}\left(h - \bar{h}\right) \quad (6)$$

Rewriting equation (5) at steady state.

$$\text{A}\,\frac{\partial \bar{h}}{\partial t} = 0 = \bar{F}\,\text{A} + \bar{F}\,\text{B} - \overline{c\sqrt{n}} \quad (7)$$

Subtracting (7) from (6) gives :

$$\text{A}\,\frac{\partial h}{\partial t} = \text{F}'\text{A} + \text{F}'\text{B}' - \frac{\bar{c}}{2\sqrt{\bar{n}}}\,\text{h}' \quad (8)$$

Where h′, FA′ , FB′ are deviations from steady state.

5. SOLUTION BY LINEARIZATION AND LAPLACE TRANSFORM

Taking Laplace transformation gives

$$\text{As h}'(\text{s}) = \text{F}'\text{A}(\text{s}) + \text{F}'\text{B}(\text{s}) - \frac{\bar{c}}{2\sqrt{\bar{h}}}\,\text{h}'(\text{s}) \quad (9)$$

$$\therefore \quad h'(s) = \frac{1}{A(s+\frac{1}{\tau})}F_A(s) + \frac{1}{A(s+\frac{1}{\tau})}F_B(s) \quad (10)$$

where $\tau = \frac{2\sqrt{\bar{h}}}{\bar{C}}A$

At steady state,

$\bar{F}_A$ = 0.015 m3/sec $\quad$ $\bar{C}_{A\,IN}$ = 2 kmol/m3
$\bar{F}_B$ = 0.005 m3/sec $\quad$ $\bar{C}_{B\,IN}$ = 1 kmol/m3
$\bar{C}$ = 0.020 m3/2 / sec $\quad$ $\bar{C}_B$ = 0.1 kmol/m3
$\bar{h}$ = 1m $\quad$ $\bar{C}_A$ = 0.14 kmol/m3
A = 1m2
since r = 2CACB
Therefore K1 = 2
Component continuity equation

$$F_A C_{A\,IN} = QC_A + K_1 C_A C_B V + \frac{d(VC_A)}{dt} \qquad (11)$$

but substituting for $\frac{dh}{dt}$ gives

$$\Rightarrow \; C_A \frac{dh}{dt} + V\frac{dC_A}{dt} = F_A C_{AIN} - QC_A - K_1 C_A C_B V \qquad (12)$$

Therefore

$$V\frac{dC_B}{dt} = F_B C_{B\,IN} - QC_B - K_1 C_A C_B V - C_B(F_A + F_B - Q) \qquad (13)$$

$$\frac{dC_A}{dt} = \left[\frac{C_{A\,IN}}{V} - \frac{\overline{C}_A}{\overline{V}}\right]F_A - \left[\frac{\overline{C}_A}{\overline{V}}\right]F_B + \left[\frac{\overline{F}_A\overline{C}_A}{\overline{V}^2} + \frac{\overline{F}_A\overline{C}_{AIN}}{\overline{V}^2} - \frac{\overline{F}_B\overline{C}_A}{\overline{V}^2}\right]V - \\ -(K_1\overline{C}_A)C_B + \left[\frac{\overline{F}_A}{\overline{V}} + \frac{\overline{F}_B}{\overline{V}} + K_1\overline{C}_B\right]C_A \qquad (14)$$

we can re-write equation 14 as

$$\frac{dC_A}{dt} = a_1F_A - b_1F_B + c_1V - d_1C_B - e_1C_A \qquad (15)$$

Similarly

$$\frac{dC_B}{dt} = -a_2F_A - b_2F_B + c_2V - d_2C_B - e_2C_A \qquad (16)$$

Taking Laplace of (15) and (16) respectively we have

$$(S+e_1)C_A(s) = a_1F_A(s) - b_1F_B(s) + c_1V(s) - d_1C_B(s) \qquad (17)$$

$$(S+d_2)C_B(s) = -a_2F_A(s) - b_2F_B(s) + c_2V(s) - e_2C_A(s) \qquad (18)$$

using equation 10, we write

$$C_A[(S+e_1)(S+d_2) - e_2d_1] = \left[\frac{a_1(S+d_2)(S+\frac{1}{\tau}) + c_1(S+d_2) + a_2d_1(S+\frac{1}{\tau}) - c_1d_1}{S+\frac{1}{\tau}}\right]F_A + \\ \left[\frac{b_1(S+d_2)(S+\frac{1}{\tau}) + c_1(S+d_2) + b_2d_2(S+\frac{1}{\tau}) + c_1d_1}{S+\frac{1}{\tau}}\right]F_B \qquad (19)$$

solving the above equation and using equation (10) and substituting the calculated values of a1 =1.86, b1= 0.14 , c1 = -0.0272, d1 = 0.28, e1 = 0.22, a2 = 0.1, b2 =0.9, c2 = 0.003, d2 = 0.3, e2 = 0.2 and 1/τ = 0.01 we have

$$C_A(S) = \left(\frac{1.86S^2 + 0.5774S + 0.05316}{(S^2+0.52S+0.01)(S+0.01)}\right)F_A - \left(\frac{0.14S^2 + 0.3406S + 0.003664}{(S^2+0.52S+0.01)(S+0.01)}\right)F_B \qquad (20)$$

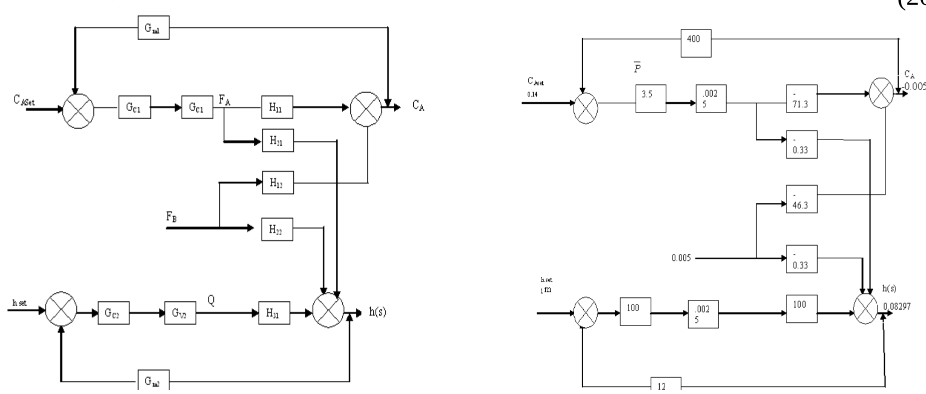


Figure 4(a) *The block diagram for the control problem. Figure 4(a) Block diagram of the feedback control loop for CSTR problem*

Transfer function of the control process for the closed loop 1 in figure 4(a) and (b) is

$$C_A(S) = \frac{H_{11}gv_1gc_1}{1+H_{11}gv_1gc_1gm_1}C_A set \quad + \quad \frac{H_{12}}{1+H_{11}gv_1gc_1gm_1}F_B \tag{21}$$

while the transfer function for the closed loop 2 is

$$h(S) = \frac{H_{31}gv_2gc_2}{1+H_{31}gv_2gc_2gm_2}h\,set \quad + \quad \frac{H_{21}}{1+H_{31}gv_2gc_2gm_2}F_A + \quad \frac{H_{22}}{1+H_{31}gv_2gc_2gm_2}F_B \tag{22}$$

These transfer functions are the controller with which we tested the behaviour of the process and hence establish the stability of the controller.

$$C_A(S) = \frac{\left[\frac{1.86(-0.035)^2+0.5724(-0.035)+0.005316}{[(-0.035)^2+0.52(-0.035)+0.01](-0.035+0.01}\right](0.0025)(3.5)}{1+\left[\frac{1.86(-0.035)^2+0.5724(-0.035)+0.005316}{[(-0.035)^2+0.52(-0.035)+0.01](-0.035+0.01}\right](0.0025)(3.5)(400)}(0.14) \quad +$$

$$\frac{-\left[\frac{0.14(-0.035)^2+0.3406(-0.035)+0.003664}{[(-0.035)^2+0.52(-0.035)+0.01](-0.035+0.01}\right]}{1+\left[\frac{1.86(-0.035)^2+0.5724(-0.035)+0.005316}{[(-0.035)^2+0.52(-0.035)+0.01](-0.035+0.01}\right](0.0025)(3.5)(400)}(0.005)$$

CA(S) = -0.0005809 (23)

$$h(S) = \left[\frac{100(0.0025)(100)}{1+100(0.0025)(12)(0.024)}\right]1 \quad + \left[\frac{\left[\frac{1}{S+0.01}\right]}{1+100(0.0025)(100)(0.024)}\right]0.015 +$$

$$\left[\frac{\left[\frac{1}{S+0.01}\right]}{1+100(0.0025)(100)(0.024)}\right]0.05$$

where S = -3.01, we have

h(S) = 0.08297 (24)

6. SIMULATION OF THE PROBLEM AND IDENTIFICATION OF OUTPUT PARAMETERS FOR NEURAL NETWORK SYSTEM

We considered a few but representative single faults which can occur during the steady- state operation of a CSTM/R when process parameters deviate by a fixed amount from their normal (or set) values. From figures 3.(a) and (b) we see the seven (7) fault parameters F1,F2,F3,C1,C2,C3 and V, but the flow rates (F) and concentrations (C) can either be high or low thus making thirteen fault pattern in all.

(i) input flow rate for Input pipe1 (F1) high
(ii) input flow rate for Input pipe1 (F1)low
(iii) input flow rate for Input pipe2 (F2) high
(iv) input flow rate for Input pipe2 (F2) low
(v) input concentration for input pipe1 (C1) high
(vi) input concentration for input pipe1 (C1) low
(vii) input concentration for input pipe2 (C2) high
(viii) input concentration for input pipe2 (C2)low
(ix) output flow rate (F3) high
(x) output flow rate (F3)low
(xi) output concentration (C3) high
(xii) output concentration (C3)low
(xiii) Volume of mixture in the CSTM/R (v_o)

We assume that these faults occur in a mutually exclusive manner. That is, only one type of fault can occur at any given time.

Table 1. *Architecture of the Network Used*.

Network used	KalKoh Hybrid Network
Learning rule	Extended Gradient descent
Transfer functions 1 and 2	Winner Takes all and Tan-Sigmoid
Learning method	Unsupervised and Supervised
No. of inputs	13
No. of output	1
No. of hidden layer	3

7. SIMULATION OF FAULTS

All the thirteen faulty process conditions were simulated separately. Each of the thirteen data sets so generated corresponds to 0.1-15% deviation (at the interval of 0.3%) from the normal value of the individual, process parameter responsible for the malfunction. Thus, each fault is represented by 150 patterns. Subsequently, all the thirteen data sets were combined to form a single input set for network training. Table 1. Shows the details of the architecture of the training network. The data structure of the resultant training input set is given in Table 2 This set can be visualized as a matrix of size (195,7) consisting of 195 fault patterns representing thirteen faults. Out of the 15 patterns of each fault covering 0.1-15% deviation range, the values corresponding to 6% and 15% deviations only are listed.

Table 2: Data structure for network training and testing

8. DISCUSSION

A controller was designed to automatically annul the effect of the disturbance FB in loop 1 so as to keep the outlet concentration of CA at a maximum point of 0.14 kmol/m3

Which is the set value (CA Set) and again to control the accumulation of material within the tank at a level of hset=1m even in the presence of disturbance from FA and FB that have direct effect on the liquid level in the tank.

The controller seeks for a deviation between CA and CAset and h(s) and h(s)set respectively. i.e. C(A)set - C(A), h(s)set – h(s). The CA obtained by our controller is consistently negative (-ve) for the problem under consideration for all values of FB input while there is no deviation in h(s) as shown on table 3.

The result obtained from the feedback control loop, CA = -0.0058093. (figure 5) shows a negative deviation which implies that our CA does not and will exceed CA set. If CA obtained is positive, summation of the deviation value plus the actual CA will result to a CA value greater than CA set. The output value of h(s) = 0.08297 shows that there is no deviation and hence the volume of the mixture in the tank remains consistent. The network result agrees with the calculated result.

To establish the stability of the controller, some inputs values for FA and FB over a range of 0% to 100% at an interval of 10% were entered. The inputs were tested the results obtained are shown on Table 3.

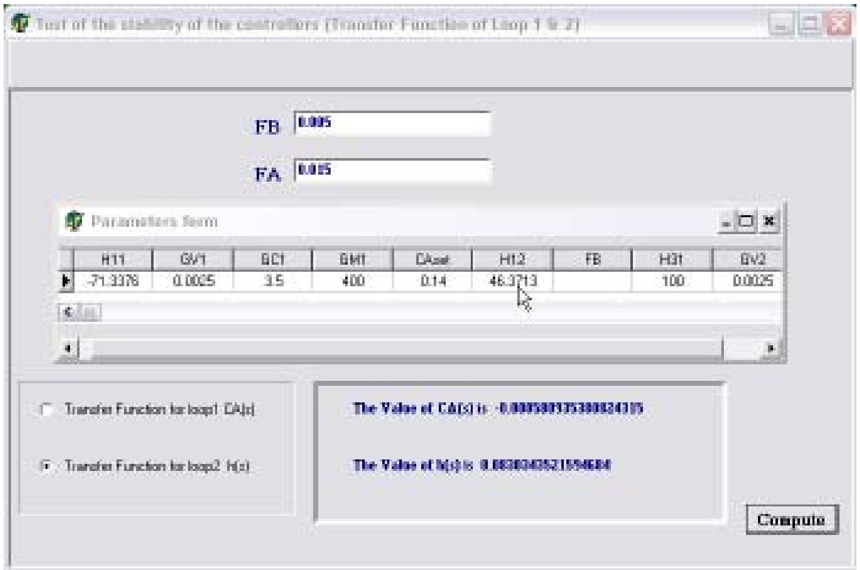


Figure 5. *The test of stability of the controller*

9. CONCLUSION

The stability of the controller system have been proved to be consistent at various level of disturbance of FB varying from 0% to 100% on CA which have been consistently below 0.1% deviation from the steady state condition. Likewise the deviation of the liquid level in the tank with aforementioned disturbance range of FB coupled with that of FA stream which was primarily meant to neutralize the effect of FB but also a form of disturbance on the liquid level have been kept at less than 10% consistently (precisely 8%) which is still tolerable. Results obtained as shown on the table 3 reveals that the concentration CA varies in a consistent manner with a negative deviation while the volume (height) of the mixture in the tank is maintained at a particular height in spite of the variations in the inlet streams. The calculated results agreed with the output of our neural network.

Conclusively we can confidently say the controller designed for the problem was stable. The Kalkoh hybrid network was successfully used to model and solve the CSTR problem keeping the system at its optimum.

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Table 2. *Controller output validating the controller's stability*

Percentage Variation (%)	FA	FB	CA	H(S)	CA (%)	H(S) (%)
0	0.0150	0.0050	-0.0058093	0.083034	0.05	8 %
10	0.0165	0.0055	-0.00674169	0.083032	0.06	8 %
20	0.0180	0.0060	-0.0007674	0.083029	0.07	8 %
30	0.0195	0.0065	-0.0008606	0.083027	0.08	8 %
40	0.0210	0.0070	-0.00095387	0.083025	0.09	8 %
50	0.0225	0.0075	-0.00104710	0.083023	0.10	8 %
60	0.0240	0.0080	-0.00114034	0.080210	0.11	8 %
70	0.0255	0.0085	-0.00123357	0.083018	0.12	8 %
80	0.0270	0.0090	-0.00132680	0.083016	0.13	8 %
90	0.0285	0.0095	-0.00140043	0.083014	0.14	8 %
100	0.0300	0.0100	-0.00151327	0.083012	0.15	8 %

Table 3: *Data structure for network training and testing*

Nature of fault	Fault Code	Training Data (Inputs)		Test Data (inputs)	
		Pattern no(s)	Deviation (%)	Pattern no(s)	Deviation (%)
Input flow rate for Input pipe 1(high)	F1H	1 – 15	(+)0.1- 15	1 – 150	(+)0.01- 15
Input flow rate for Input pipe 1 (low)	F1L	16 – 30	(-)0.1- 15	151 – 300	(-)0.01 - 15
Input flow rate for Input pipe 2 (high)	F2H	31 – 45	(+)0.1- 15	301 – 450	(+)0.01- 15
Input flow rate for Input pipe 2 (low)	F2L	46 – 60	(-)0.1- 15	451 – 600	(-)0.01 - 15
Input concentration for input pipe 1(high	C1H	61 – 75	(+)0.1- 15	601 – 750	(+)0.01- 15
Input concentration for input pipe 1 (low	C1L	76 – 90	(-)0.1- 15	751 – 900	(-)0.01 - 15
Input concentration for input pipe 2 high	C2H	91 – 105	(+)0.1- 15	901 – 1050	(+)0.01- 15
Input concentration for input pipe 2 (low	C2L	106 – 120	(-)0.1- 15	1051 – 1200	(-)0.01 - 15
output flow rate high	F3H	121 – 135	(+)0.1- 15	1201 – 1350	(+)0.01- 15
output flow rate low	F3L	136 – 150	(-)0.1- 15	1351 – 1500	(-)0.01 - 15
output concentration high	C3H	151 – 165	(+)0.1- 15	1501 – 1650	(+)0.01- 15
output concentration low	C3L	166 – 180	(-)0.1- 15	1651 – 1800	(-)0.01 - 15
Volume of mixture in the CSTM	V	180 – 195	(+)0.1- 15	1801 – 1950	(+)0.01- 195