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Adaptive Neuro-Fuzzy Inference System for Effect of Wall Capacitance in a Batch Reactor

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Abstract

Runaway may occur in a chemical reactor when a small change in one of the operating variables such as feed or coolant temperature, flow rate, concentration etc. causes a large increase in the reactor hot spot or exit temperature. This may lead to an accident or an explosion, which results in damage to men, machines and materials. In the present work, acid catalysed hydrolysis reaction of acetic anhydride in presence of acetic acid as solvent and sulfuric acid as catalyst is chosen as reaction system. In this paper, I have tried to show, how successfully Adaptive Neuro-Fuzzy Inference System (ANFIS) is used for finding the effect of wall capacitance in a batch reactor. The simulation experiments indeed demonstrate the effectiveness of the proposed method.

Keywords: Adaptive Neuro-Fuzzy Inference System (ANFIS), Batch-Reactor, Wall Capacitance.

I. Introduction

Much of the human knowledge is vague and precise. Often,Human thinking and reasoning involve inexact information. The sources and the nature of inexact information may be different for different problem domains. The fuzzy inference system (FIS) is a popular computing framework based on the concepts of fuzzy set theory , fuzzy if – then rules and fuzzy reasoning. It has found successful applications in a wide variety of fields, such as automatic control, time series prediction, Digital signal processing, Bio-medical engineering, Robotics etc. It is also known by other names like fuzzy rule base system, fuzzy associative memory, fuzzy logic controller and simply fuzzy system. The control of nonlinear processes like bioreactors does not give satisfactory responses by conventional PI controller.

II. Fundamental fuzzy system concepts and fuzzy logic

Fundamental fuzzy systems concepts include the following:

(1) Linguistic variables.
(2) Fuzzy sets.
(3) Types of fuzziness.
(4) Membership functions.
(5) Linguistic variables and label.
(6) Fuzziness procedure.
(7) Fuzzy Rules
(8) Computational rules of inference (CRI).
(9) De-fuzzificationprocedure.

Fuzzy set theory provides a formal system for representing and reasoning with uncertain information. In this system, set membership is not “all or nothing”, but rather is defined via non binary membership function. In practice, “fuzzy rules” encapsulate approximate relationships between observations and response or input and output in control applications.

The essential characteristic of fuzzy logic is as follow:

(1) In fuzzy logic, exact reasoning is viewed as a limiting case.
(2) In fuzzy logic, everything is a matter of degree.
(3) In fuzzy logic, inference is viewed as the process of propagation of elastic constraints.
(4) In fuzzy logic, and logical system can be fuzzified.

In conventional or crisp sets an element ‘x’ is either a member of a set ‘s’ or not. Thus, the membership function (MF) for a crisp set ‘s’ is a binary valued function (i.e either 0 or 1). Fuzzy sets generalize the notion of crisp sets, as defined in the previous section. In fuzzy realm, membership functions are no longer binary valued, and it is therefore meaningless to try to simply indicate membership in a set. In crisp set, membership is dichotomous (“yes or no”), whereas in fuzzy set we allow the concept of graded membership (“more – or – less”).

Fuzzy Inference is the process of formulating, the mapping from a given input to an output using fuzzy logic. The mapping then provides a basis from which decisions can be made, or patterns discerned. The process of fuzzy inference involves all of the pieces membership functions, fuzzy logic operators, and if-then rules.

There are two types of fuzzy inference systems that can be implemented in the Fuzzy Logic Toolbox: Mamdani-type and Sugeno-type.

III. Major components of a fuzzy system

As shown in figure:1, the general structure of a system employing fuzzy concepts consists of a member of entities, some of which are optional. These includes an interface, which may allow both fuzzy and crisp inputs, A crisp – fuzzy interface which converts non-fuzzy (crisp) inputs in to their fuzzy counterparts, may be involved. A fuzzy computational mechanism, which processes fuzzy sets through fuzzy rules, finally an optional “de-fuzzification” Interface, which converts the fuzzy domain results in to non fuzzy (crisp) outputs as shown.

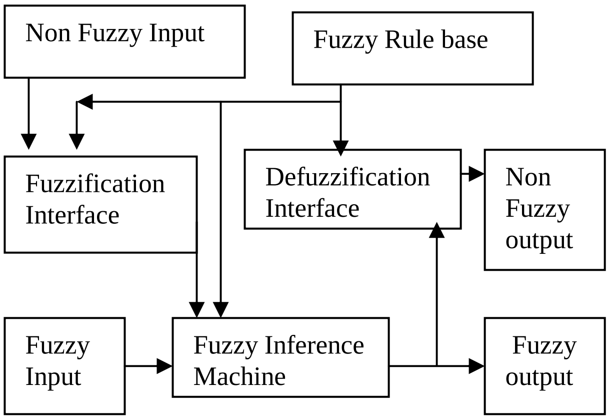

Figure 1: Fuzzy system architecture for control.

IV. Fuzzification and De-fuzzificatioN

System inputs are assumed to occur as the output of sensors, thus, a single number for each problem variable must be converted in to the fuzzy domain for each linguistic label. Given the appropriate membership functions, this conversion involves mapping the input variable to a fuzzy set membership value.

Defuzzification is necessary in order to provide crisp output signals. For example, in a control application, the output of the fuzzy controller must be an exact voltage, current, flow setting etc. We can not except physical systems to be able to “speed up slightly” (a fuzzy concept) ; rather , the controller must specify “ speed = 25 ips” .

V. ANFIS For A Batch-Reactor: Constant Coolant Flow Rate and Heat Loss Experiment

In the present work, the hydrolysis reaction of acetic anhydride in the presence of sulfuric acid as catalyst is studied. Acetic acid is used as a solvent to have a homogenous reaction mixture. The hydrolysis reaction of acetic anhydride can be written as,

$$(CH_3CO)_2O + H_2O \xrightarrow[CH_3COOH\ (SOLVENT)]{H_2SO_4\ (CATALYST)} 2(CH_3COOH)$$

Water is taken in excess so that pseudo – first order kinetics can be obtained. The initial concentration of reactants and that of solvent are (at instant time t = 0),

Acetic Anhydride	=	5.0 gm mole / lit,
Water	=	18.61 gm mole / lit,
Acetic Acid	=	0.3270 gm mole / lit,
Sulfuric Acid	=	0.057 gm mole / lit.

VI. Mathematical Modeling

The following assumptions are made in the development of the mathematical model for a batch reactor.

(1) The specific heat of the reaction mixture can be calculated as the weight fraction weighted mean of individual component specific heat.
(2) The reactor wall, being thin (about 0.5 mm) can be assumed to be at a uniform temperature equal to the reactor temperature.
(3) The density of the reaction mixture can be calculated by using the following equation:
$1 / \rho = \sum wi / \rho i$

Where,
wi and ρi are the weight fraction and density of the spaces i.

Based on the above assumptions, the mass and energy balance equations for a transient unsteady batch reactor can be written as:

$$dNA / dt = -k\ NA = rA$$

$$(V\rho\ CP + Ws)\ dT / dt = (-\Delta H)\_rA\ V - UA\ (T - Tci)$$

Where,
NA is number of moles of acetic anhydride at any instant time, g moles,
K is first order rate constant , min^{-1},
V is volume of the reactor, 318 ml^3,
T is temperature of the reactor at any instant time, °C,
Ws is the wall capacitance, (38.4 cal / °C).

VII. Table 1: Constant Coolant Flow Rate Experiment In a Batch Reactor. Flow rate qc= 60 cc/min.

Time Sec	**Experimental Temperature Degree Celsius**
0	28
30	28.5
60	29
90	30.4
120	31.6
150	33
180	34.4
210	36
240	38.2
270	40.3
300	43.7
330	49.5
360	65.5
390	80.3
393	84.1
420	72.1
450	65.6
480	60
510	55.3
540	51.3
570	49.3
600	47

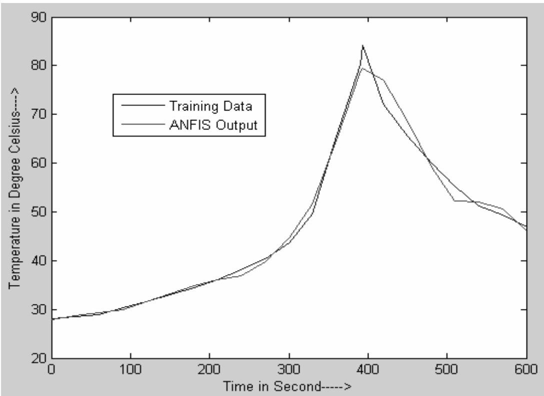

Figure 2: ANFIS Result For Time versus Temperature.

ANFIS info:
Number of nodes: 24
Number of linear parameters: 10
Number of nonlinear parameters: 15
Total number of parameters: 25
Number of training data pairs: 22
Number of checking data pairs: 0
Number of fuzzy rules: 5

Start training ANFIS ...

1 1.96454
2 1.96115
3 1.95779
4 1.95447
5 1.95117
Step size increases to 0.011000 after epoch 5.
6 1.9479
7 1.94433
8 1.9408
9 1.93731
Step size increases to 0.012100 after epoch 9.
10 1.93385
11 1.93008
12 1.92636
13 1.92268
Step size increases to 0.013310 after epoch 13.
14 1.91904
15 1.91508
16 1.91117
17 1.9073
Step size increases to 0.014641 after epoch 17.
18 1.90349
19 1.89935
20 1.89527

Designated epoch number reached --> ANFIS training completed at epoch 20.

VIII. Conclusion

The effect of the wall capacitance is verified for W_S = 10, Where, Time versus Concentration graph is decaying and control is achieved after 4 second interval. W_s = 238.5, Where Time versus Concentration graph is a straight line and control is achieved at the instant. and W_S = 239, Where, Time versus Concentration graph is increasing i.e. it is similar to first order system and control is achieved after 3.5 second interval. (For V= 318 , ρ = 0.995 and CP = 0.8, flow rate qc= 60 cc/min)

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