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Fuzzy Temperature Control in a Batch Polymerization Reactor Using ANFIS Method

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***Abstract*—In this paper a Sugeno-Type FLC for temperature control in a batch polymerization reactor is developed and tested through a simulation study. A novel ANFIS-based method is implemented to design a practicable advanced controller. Temperature of a pilot-scale jacketed batch reactor is controlled by manipulating the reactor cooling water temperature. Manifest feature of the proposed method is smoothing of undesired control signal of conventional PI controller. The simulation study shows that the proposed controller has good set point tracking and disturbance rejection properties. Also it is robust against changes in the system parameters. It is also superior to the conventional PI controller and even previously proposed advanced controllers.**

***Index Terms*—ANFIS, Batch Polymerization Reactor, Fuzzy Logic Controller (FLC), Practicability Constraints.**

I. INTRODUCTION

It is well-known fact that batch process is gaining wider ground in chemical industries, owing to its availability and operational flexibility. Compared with continuous processes the control of batch processes is more difficult and thermal runaway would cause a runaway reaction [1], because physical and chemical properties of the contents, such as heat capacity, heat transfer coefficient and reaction rate vary from run to run and within runs [2].

The main control objective of the industrial batch polymerization reactor operation is to maintain or to track desired trajectories for reactor temperature. The importance of temperature control during polymerization reaction is due to its effects on polymer properties such as average molecular weight (MW) and molecular weight distribution (MWD). These properties are straightly related to the physical and mechanical polymer qualities and its commercial applications.

The suspension polymerization of styrene in batch reactor kinetics is assumed to follow the free-radical mechanism and this batch reaction is considered a challenge for process control design, presenting nonlinear and transient behavior. A major source of non-linearity is due to the autocatalytic nature of the polymerization reaction (known as gel effect). It may lead to uncontrollable situations, resulting in excessive temperature rise, rapid increase in polymerization rate and equipment plugging.

Viscosity raise also affects negatively the heat removal, because it leads to a decrease in the effective heat transfer coefficient between the reactor wall and the cooling water in the jacket [3]. Temperature control of batch polymerization reactor has attracted attention in recent years [3-11]. In some cases both of temperature behavior and control action are remarkably oscillatory at the end of the batch period [12-16]. Despite considerable research efforts in developing new methods for modeling and control of nonlinear systems over the last decade, many of these advanced techniques have not found applicability in real industrial problems. According to available survey of advanced control for batch polymerization reactors [15], there is a huge gap between industry and research practices. This is primarily due to high implementation costs and the lack of theoretical knowledge required to understand these sophisticated methods and computational burden of these methods. Secondly most of the time the practical constraints didn't take into account. Therefore, there is an increasing awareness of the need for practical approaches to aid engineers to better understand and perform complex modeling and control tasks [17]. Incorporating actuation constraints is a brilliant idea that can be observed in few works like [18]. In the present work, we tried to develop a practicable controller by taking some practical constraints into account. Firstly, a conventional PI controller is designed, which is widely used in industry [19]. Since the obtained control signal had abrupt changes, which can't be produced practically. Then a Sugeno-type FLC (Fuzzy Logic Controller) is developed. The input/output data set of the existing PI controller used to train an ANFIS. The adaptive-neuro fuzzy inference system (ANFIS) will help us to produce a smooth and practicable control signal. Removal of the heat of polymerization reactor is accomplished by circulating coolant through a jacket [20]. The paper focuses on the temperature control of a polystyrene batch reactor with rule based Takagi-Sugeno fuzzy controller with ANFIS Method. So its sections arranged as plant description including kinetics model and model formulation, control strategy, result and discussion and at last conclusion.

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II. PLANT DESCRIPTION

A. Kinetics Model

The kinetic mechanism of styrene is a free radical

mechanism (Table 1) which consists of four main elementary steps, i.e. initiation, propagation, chain transfer, and termination. The decomposition of the initiator, an azo or peroxide compound, follows first order kinetics. The initiator radical can react very rapidly with a monomer molecule to form a monomer radical and sometimes it disappears by side-reactions: the initiator efficiency factor f is the fraction of initiator radicals reacting in the desired reaction. Kinetics data were taken from the literature [1]:

$$K_i = 1.7\times10^{14}\exp(-15103/T) \quad [s^{-1}] \tag{1}$$

$$\bar{K}_i = 2.19\times10^{5}\exp(-13810/T) \quad [m^6Kmol^{-2}s^{-1}] \tag{2}$$

$$K_p = 1.09\times10^{7}\exp(-3548/T) \quad [mol^3Kmol^{-1}s^{-1}] \tag{3}$$

$$K_{tM} = 1.09\times10^{4}\exp(-3548/T) \quad [mol^3Kmol^{-1}s^{-1}] \tag{4}$$

$$K_{tc} = K_{tc}^{0} g_t \tag{5}$$

$$K_{tc}^{0} = 1.7\times10^{9}\exp(-1141.42/T) \quad [mol^3Kmol^{-1}s^{-1}] \tag{6}$$

$$\ln(g_t) = -0.1104x - 6.362x^2 - 0.1704x^3 \tag{7}$$

See appendix A for nomenclature. Assuming that the auto-initiation rate of styrene polymerization is second-order initiation, component balances are defined as follows [1]:

$$\frac{d[I]}{dt} = -K_i[I] \tag{8}$$

$$\frac{d[M]}{dt} = -\left\{2fK_i[I] + 2\bar{K}_i[M]^2 + (k_p + K_{tM})[M][R]\right\}$$

$$\text{at } t = 0,\ [M] = [M]_0 \tag{9}$$

$$\frac{d[P]}{dt} = K_{tM}[M][R] + \frac{1}{2}K_{tc}[R]^2 \quad \text{at } t = 0,\ [P] = 0. \tag{10}$$

For a batch reactor of suspension polymerization, heat balance is defined as follows [1]:

$$(rC_pV)_S \frac{dT}{dt} = (-\Delta H_p)V_{MP}K_p[M][R] - UA(T - T_c)$$

$$at\ t = 0,\quad T = T_0 \tag{11}$$

Only styrene, polystyrene, and water are assumed to have significant volumes. The volumes of other compounds (initiator, suspending agents, etc.) are assumed to be negligible. The volume of the reactants (VMP) is calculated as a function of the reactor temperature and the monomer conversion (x). It is defined as follows:

$$V_{MP} = \frac{m_M^0}{(1-x)r_M(T) + xr_p(T)} \tag{12}$$

$$x = \frac{[M]_0 - [M]}{[M]_0} \tag{13}$$

The accumulated heat ((ρCpV)s) is defined as follows:

$$(rC_pV)_s = [(1-x)C_{pM} + xC_{pP}]m_M^0 + m_WC_{pW} \tag{14}$$

At the initial time of reaction, as heat of generation is negligible, heat balance is defined as follows:

$$(rC_pV)_s \frac{d[T]}{dt} = U_0A(T - T_c) \tag{15}$$

An initial overall heat transfer coefficient (U0) can be calculated by integrating Equation (16). But the overall heat transfer coefficient is varied while the reaction progresses because heat of generation is no more negligible and physical and chemical conditions of reactants, i.e. viscosity etc., are varied. Therefore, the viscosity of the reacting mixture (hydrophobic phase) increases significantly and the heat transfer coefficient decreases sharply with conversion. In this paper, the overall heat transfer coefficient has been modeled through the use of empirical correlation proposed by Takamatsu et al. (1988). The overall heat transfer coefficient is defined as follows:

$$U = U_0\left[1 - a\ \exp(1 - \frac{1}{x})\right] \tag{16}$$

TABLE 1: REACTION MECHANISM OF FREE RADICAL POLYMERIZATION

Initiation :

Decomposition of the initiator :

$$I \xrightarrow{K_i} I^*$$

Chain starts by initiator radical :

$$I^* + M \rightarrow R_1$$

Auto – initiation :

$$M + M \xrightarrow{\bar{K}_i} 2R_2$$

Pr*opagation* :

$$R_i + M \xrightarrow{K_P} R_{i+1}$$

*Ter*min*ation by combination and disproportionation* :

$$R_i + R_j \xrightarrow{K_{tc}} P_{i+j}$$

$$R_i + R_j \xrightarrow{K_{td}} P_i + P_j$$

Chain transfer to monomer and agent :

$$R_i + M \xrightarrow{K_{tM}} P_i + R_1$$

$$R_i + S \xrightarrow{K_{tS}} P_i + R_0$$

B. Reactor Model

To simulate thermal behavior of suspension polymerization of styrene in a batch reactor, we assumed that heat of generation was negligible at the initial time of reaction, the volume of additive agents (initiator, suspending agents, etc.) were negligible and physical and chemical conditions of additive agents were negligible, too. Having the mentioned 4 non-linear differential equations (i.e. Equations 8 to 11) One can make a Simulink® model that takes coolant temperature (T_c) as its single input and gives back reactor temperature (T) as its single output (Fig. 1), but first some constants and initial values must be assigned.

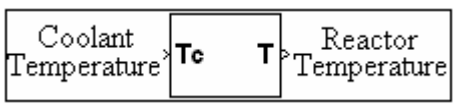

Fig. 1: Batch reactor simulated by Simulink®

So this model takes initial data, i.e. monomer weight (mM), initiator weight (mi), water weight (mW), reaction temperature (T0), cooling temperature (Tc), initial overall heat coefficient, initial heat transfer area (A0), and initiator efficiency (f), etc. Then it calculates resulting data including concentrations of monomers ([M]), initiator ([I]), and radicals ([R]), overall heat coefficient, heat transfer area (A), conversion (x), kinetics, etc. The used literature data of physical and chemical conditions of materials as follows [1]:

Styrene:

$$r_M[kg/m^3] = 924 - 0.981(T - 273.15)$$

$$C_{pM}[kJ/kgK] = 1.547 + 4.308\times10^{-3}(T - 273.15)$$

Polystyrene:

$$r_p[kg/m^3] = 1084 - 0.605(T - 273.15)$$

$$C_{pP}[kJ/kgK] = 1.225 + 4.04\times10^{-3}(T - 273.15)$$

Water:

$$r_W[kg/m^3] = 1001.23/(1.257 - 1.9625\times10^{-3}T + 3.77\times10^{-6}T^2)$$

$$C_{pW}[kJ/kgK] = 5.442 - 8.186\times10^{-3}T + 1.307\times10^{-5}T^2$$

$$Polymerizationheat: (-\Delta H_p) = 73200\,kJ/kmol$$

The estimated temperature profiles were in good agreement with experimentally measured values [1]. Therefore the control design can base on this model of batch polymerization. For [I]0=0.0716 step response of the system is as shown in Fig. 2.

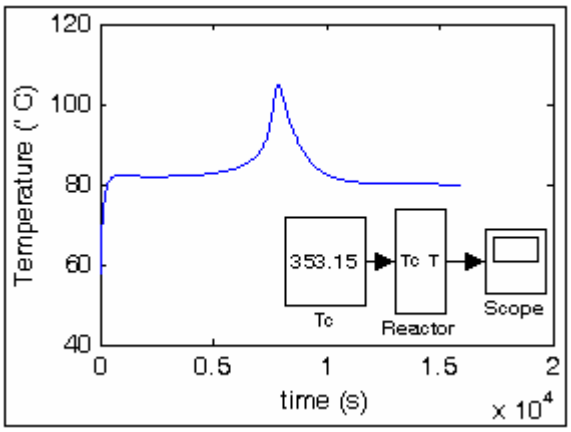

Fig. 2: Step response of the batch reactor for [I]0=0.0716

III. CONTROL STRATEGY

It is well known that the temperature control of the reactor depends mainly on the heating and cooling system of the reactor. A jacketed reactor temperature control is ensured by acting on both variables of the flow rate of cooling water and temperature of the coolant. Most often, one of these two input rates is fixed and the other is changed as manipulated variable [4]. In this work, the fluid flow rate was set to a mean value and removal of the heat of polymerization is accomplished by circulating coolant through a jacket (Fig. 3), while only temperature of coolant is adjusted.

Adaptive neural network based fuzzy inference system (ANFIS) is an intelligent neuro-fuzzy technique used for modeling and control of ill-defined and uncertain systems. ANFIS is based on the input–output data pairs of the system under consideration [21].

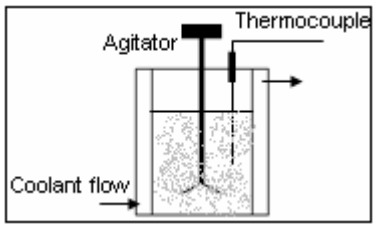

Fig. 3: A jacketed batch reactor

The algorithm of the ANFIS method has been defined by Jang et al. [22]. It has attained its popularity due to a broad range of useful applications in such diverse areas in recent years. The adaptive network based fuzzy inference system (ANFIS) represents a useful neural network approach for the solution of function approximation problems. Data driven procedures for the synthesis of ANFIS networks are typically based on a training set of numerical samples of the unknown function to be approximated. Since introduction, ANFIS networks have been successfully applied to classification tasks, rule-based process controls, pattern recognition problems and the like [21]. Here, just like what happens in industry, a conventional PI controller is used to track the predetermined set point. From the literature [19], PI parameters can be set as P+ Is = 16+0.425I to achieve best performance. Despite of good set point tracking (Fig. 4) such a controller will produce an undesirable control signal with abrupt changes (Fig. 5). It is practically impossible to manipulate a coolant liquid's temperature with a rate greater than 10 'C/min, on the other hand manipulated variable signal doesn't have the permission to overrun beyond some extents. Because it may vaporize the coolant water, and then previously achieved equations aren't valid any longer. Solving the former problem imposes high cost and sophisticated devices, while the later enforces us to use some expensive and rarely available oils instead of water. So we aimed to propose a controller witch produces a smooth and practicable control signal and also can perform with cheap and available coolants like water.

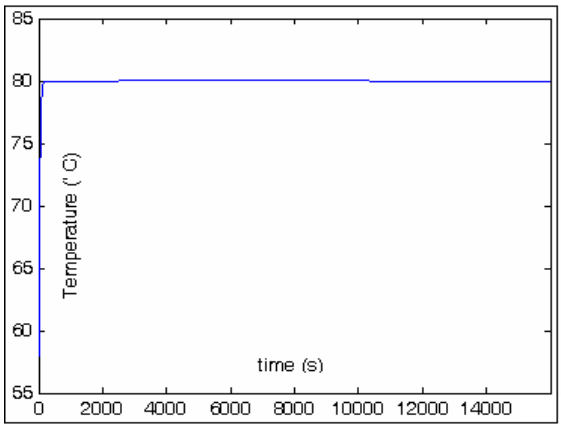

Fig. 4: Set point tracking property of PI controller

The main idea is to use the input/output of PI controller as a training data set for an ANFIS. The ANFIS will mimic PI controller all over the process, except in cases the control signal has abrupt variations. Therefore newly obtained system can perform acceptable, while attenuates the amplitude of the former signal and doesn't include abrupt variations in manipulator signal.

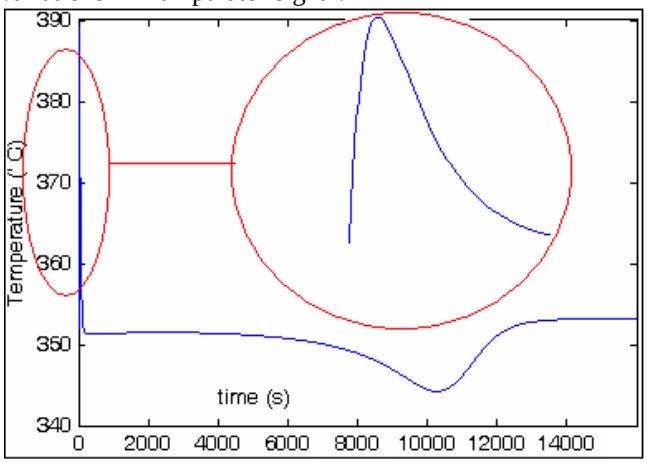

Fig. 5: Undesirable control signal required for PI controller

Using ANFIS editor GUI it is found out the best possible configuration is as follows: The controller developed in this way, uses just three simple rules based on 3 linguistic variables defined over the input universe of discourse. (Fig. 6)

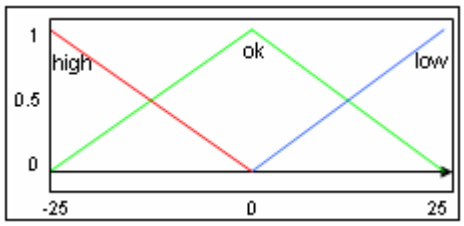

Fig. 6: Input membership functions

1. If (input1 is ok) then (output is M)
2. If (input1 is low) then (output is H)
3. If (input1 is high) then (output is L)

Output membership functions are set constants corresponding to the L (low), M (medium), and H (high). (Fig. 7)

we aim to manipulate a temperature as our control lever, it is clear that the temperature should vary between 0 and set point (353 'K), but in the case of medium level, two points are considerable: firstly, initial temperature of the reactants is about 333 'k and secondly, maximum reactor temperature in an open loop system (Fig. 2) is about 383 'K. So it seems sensible to set the mean value equal to 353 'K. One could find a simple semantic relation between rules and desired control action. For example if error signal has a large positive value (i.e. input one is low), it indicates the reactor temperature is low, so control action should increase to pull up the temperature and so forth. Furthermore, nonlinear relation between input and output of proposed ANFIS is visualized in Fig. 8.

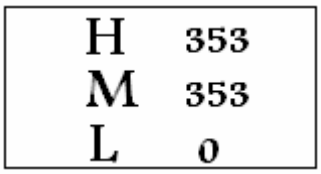

Fig. 7: Output membership functions

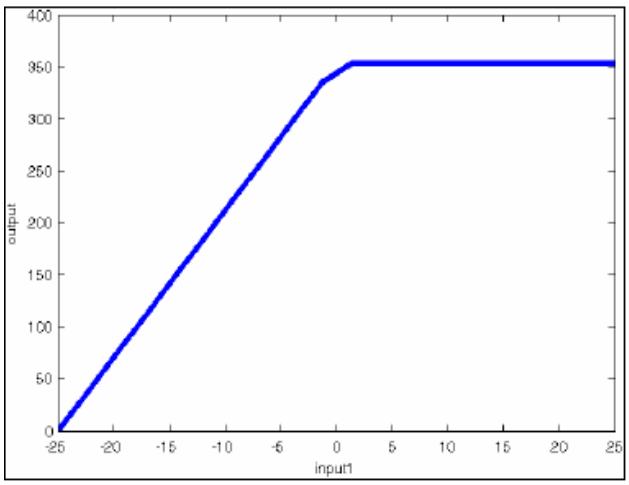

Fig. 8: Non-linear relation between input and output of proposed ANFIS

IV. Results and Discussion

Presented controller is used in a conventional configuration (Fig. 9) to be tested. As can be seen in Fig. 10 the controller leads to an acceptable set point tracking and elegant control signal. The claim is supported by maximum variations of 9 ' C and maximum slope of 1.7 'C/min in the obtained control signal. So it is practicable and implementable by low cost device and material. Also the quality of product is guaranteed by the maintenance of reactor temperature at desired point all over the batch. The controller also shows robustness against system parameter variation.

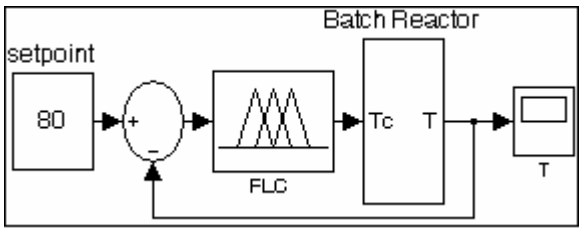

Fig. 9: Proposed FLC configuration

The most likely to change and most damaging parameter is the initial concentration of initiator $[I]_0$. Increase of this parameter from 0.0716 to 0.18 (more than 2.5 times) makes the gel effect more violent and also it takes place faster in a batch. As can be seen in Fig. 11-(a) the overshoot in step response raises from 107 (Fig. 2) to 135 'C. Such a mistake is likely to happen, but the proposed controller can bridle such a dangerous state. System step response for $[I]_0$= 0.18 and the controller performance are shown in Fig. 11. The most considerable part of this work is paying special attention to practicability constraints. Considering these constraints and presenting a simple and efficient controller make us hopeful to attain applicability in real industrial problems. Low cost, simple structure, smooth and practicable control signal

guaranties applicability of proposed controller. It seems such properties would suffuse the huge gap existing between industry and research practices [15].

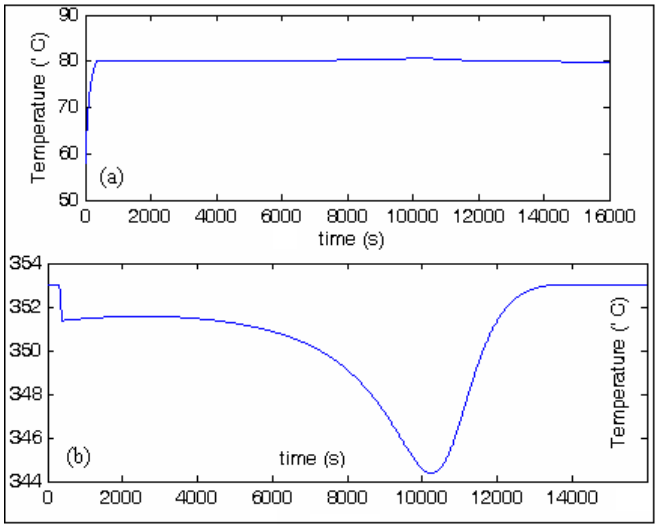

Fig. 10: Proposed FLC performance, a) set point tracking b) smooth control signal

V. Conclusion

Temperature control in a batch reactor is of high importance, because it effectively affects the product properties and quality. Commonly used PID controllers, can't perform on systems which include varying parameters, on the other hand advanced controllers which have been proposed in literature, due to complexity and computational burden, necessitating high cost and ignoring some practical constraints haven't been applied yet. In this study a simple Sugeno-type FLC was developed and tested on a batch polymerization reactor. Design approach had two stages, designing PI controller and smoothing its control signal using ANFIS. Using input/output set of the PI controller as a training data set, an ANFIS is trained to function instead of former controller. The controller presents good set point tracking properties and robustness against system parameters variation. It also requires a smooth and practicable control signal. For future works, tracking some multilevel temperature profiles (as is common for some batch processes) and solving the actuation delay time problem, can be investigated.

Appendix A: Nomenclature

A = surface area of heat transfer [m^2]

C_P = specific heat capacity [$J\,kg^{-1}K^{-1}$]

I = initiator molecule [-]

I^* = initiator radical molecule [-]

$[I]$ = concentration of initiator [$kmol\,m^{-3}$]

k_i = rate constant of initiator decomposition [s^{-1}]

$\bar{k}_i$ = rate constant of initiation [$m^6\,kmol^{-1}\,s^{-1}$]

k_P = rate constant of propagation [$m^3\,kmol^{-1}\,s^{-1}$]

T_c = temperature of the jacket or coolant [K]

t = time [s]

U = overall heat transfer coeff. [$kJ\,m^{-2}\,s^{-1}\,K^{-1}$]

V = total suspension vol. of reacting mixture [m^3]

V_{MP} = volume of reacting mixture [m^3]

x = conversion [-]

a = constant defined in Equation 16 [-]

r = density [$kg\,m^{-3}$]

k_{tc} = rate constant of termination by combination [$m^3\,kmol^{-1}\,s^{-1}$]

k_{tM} = rate constant of chain transfer to monomers [$m^3\,kmol^{-1}\,s^{-1}$]

M = monomer molecule [-]

$[M]$ = concentration of monomers [$kmol\,m^{-3}$]

m = weight [kg]

P_i = dead polymer with i monomer unit [-]

$[P]$ = concentration of polymers [$kmol\,m^{-3}$]

R_i = free radical molecule with i monomer unit [-]

$[R]$ = concentration of radical [$kmol\,m^{-3}$]

T = temperature of the reactor K or ^oC]

⟨Subscript⟩

I = initiator

M = monomer

0 = initial

P = polymer

S = suspension

W = water

⟨Superscript⟩

0 = initial

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