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Nonlinear Observer-Based Online Optimal Control for Batch Reactor Using Particle Swarm Optimization

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ABSTRACT

An exothermic batch reactor emits a large amount of heat rapidly during its reaction. It is creating a suitable temperature controller is a challenging task. Exothermic activity speeds up the reaction rate and releases more heat. As a result, insufficient temperature control may cause the reaction to become unstable, threatening plant personnel and equipment. Thus, a particle swarm optimization algorithm (PSO)-based online optimal temperature management approach for an exothermic batch reactor is proposed as a modern intelligent control. PSO is used to get the ideal reaction temperature for the batch reactor type offline, maximizing the intended product. Additionally, online PSO is used based on the nonlinear generic model control (GMC) parameters according to the cost function to achieve the best performance for temperature management of the nonlinear batch reactor. An online nonlinear state estimation is created for the batch reactor's reacting component concentrations. This nonlinear estimator is proven to match to the true state, assuring the stability of the nonlinear batch reactor controller system and saving the cost. The simulation results show the effectiveness and high performance of the suggested controller. Additionally, the robustness of the proposed controller is assured by showing zero steady state error and zero overshoot although the changes of the operational and process parameters with high rate of ±30% and -40% for the reference exothermic batch reactor type.

1. INTRODUCTION

A batch reactor is a type of chemical reactor that is used in practically processing units or plants. The batch production method is widely used and has held an especially strong position in recent decades until it meets the needs of market development [1]. Because so much heat is produced as soon as the reactants are mixed together, temperature control in an exothermic batch process—a unique kind of batch reactor has always been challenging [2]. The process temperature will rise and the reaction rate will quicken due to the released heat. More heat is produced as a result, which could cause the reaction to become unstable. Personnel and equipment at the plant could be seriously endangered by thermal runaway caused by an inefficient control system. [3].

Batch reactor control has generally encountered formidable obstacles. Due to their inherent complexity, which is demonstrated by many researchers [4&5], batch reactors have the following characteristics: (i) highly nonlinear behavior because reaction rates depend on concentrations and temperature; (ii) time-varying system, meaning that process variables and parameters change over time; (iii) lack of steady state operating conditions; (iv) imperfect model; (v) complex kinetic reactions that occur in batch reactors are also rarely understood; and (vi) expensive cost of measurement data such as (concentration) where the high cost of online sensors for measurement the concentration of the materials in the batch reactor that makes it challenging to directly manage a product's properties [5]. Only a small number of physical variables, like temperature and pressure, may be measured directly online.

There are many research methods applied their controllers on linearized models of batch reactors such as; M. S. Alhajeri et.al [6] suggested linear model predictive control (LMPC), and Guojun et.al [7] produced three simple models of the dynamic batch reactor utilizing Linearization technique then applied nonlinear model predictive control (NMPC). Also I.D. Gil et al. [8] suggested a nonlinear geometric controller based on input/output linearization to temperature control. But the controller based on a linear model for the batch reactor management does not ensure sufficient performance for practical implementation. So, recent research studies are mostly concentrated on nonlinear model-based control techniques such as; [9, 10] nonlinear model predictive control (NMPC), [11] (NMPC) and Sliding Mode controls.

Among these advanced control systems, a generic model control (GMC) technique is one of the most investigated control algorithms. This is because nonlinear process models do not need to be linearized as they may be directly interpreted in the GMC control algorithm. Moreover, compared to other model-based control methods, its implementation is comparatively simple; as a result, this control technique is applied in many chemical processes especially for batch reactor such as in [12-15].

Practical implementation of effective controller of batch reactor depends on measurements accuracy or estimations of the states of the process. Concentrations of raw components and products of the batch reactors are the main states of the process. The main challenge is the difficulty of high cost of online concentration sensors. Most research use the exothermic batch reactor type explained in [14] did not mention online estimation for its main states. For example, [14] estimated the parameter heat released by the reaction online using a three-term difference equation and an exponential filter. and by [15] applying neural network estimator. [7] used extended kalman filter (EKF) for estimating the parameters heat release by reaction and rate of one reaction. A basic contribution in this work is discussed a nonlinear online estimation of main states of the batch reactor type based on only one concentration sensor and one temperature sensor based on theoretical basics of nonlinear observer design descried in [16].

Because batch reactors create a wide range of valuable chemicals, there is a lot of interest in optimizing batch operation to create products of exceptional quality and purity while eliminating unwanted products. There has been a lot of discussion in the literature on the use of process optimization in batch reactor control. [1, 3, 13]. Optimal control of batch reactor can be for identifying an ideal set point of reaction temperature giving the maximum desired product [17] or and get the best values of the required control system[13-15]. PSO is one of the most effective techniques for fixing optimization issues. It has shown to be active in resolving problems involving nonlinearity and non-differentiability, multiple optima, high dimensionality, and furthermore, it is relatively simple [18].

The aims of this work are; (a) designing an effective nonlinear controller achieved the optimal operating

temperature that gives maximum desired product for the exothermic batch reactor, (b) achieving the real time controller by designing online nonlinear observer that estimate the main states with minimizing the cost and assuring the stability of the system. In this context, firstly PSO is implemented to obtain an ideal operating temperature that maximizing desired product of the exothermic batch reactor presented by [14]. Then, using the obtained optimal operating temperature as step point to optimize the parameters of nonlinear controller GMC by implementing PSO. After, an online estimator is constructed using only one online concentration sensor that to achieve reducing of the cost. Also, this nonlinear observer is designed with a guarantee of the stability of the suggested nonlinear controller batch reactor system. Furthermore, the flexibility of the proposed temperature controller is examined by saving its high performance although changing the operating parameters of the reactor model with high rates.

2. PARTICLE SWARM OPTIMIZATION

PSO is an intelligent technique that mimics a flock of birds or a school of fish looking for food [18]. One of the most effective techniques for fixing optimization issues is this one. It is a rather straightforward and has been demonstrated to be effective in resolving issues with nonlinearity and non-differentiability, numerous optima, and high dimensionality [19]. The PSO algorithm as shown in figure (1) makes the assumption that the search space is filled with a population of particles that move randomly in search of the optimal answer. Each particle has a location and velocity vector, and each position coordinate corresponds to a set of variables that can be adjusted to obtain the best cost function value for the situation. At each time step, each particle manipulates itself to achieve the best individual X_{PB} and global X_{GB} placements relative to its neighbors using a random weighted acceleration. The velocity and position of the particle are adjusted using the following equations [20, 21]

$$v_{(i+1)} = w.v_i + C_1.rand_1().(X_PB - X_i) + C_2.rand_2().(X_GB - X_i)$$
 (1)

$$X_{i+1} = X_i + v_{i+1}$$
(2)

Where: rand₁() and rand₂() are two random values in the range [0, 1], $C_1 \& C_2$ are the acceleration constants, and w is the inertia weight factor. The inertia weight factor w and acceleration constants $C_1 \& C_2 2$ employed in this investigation are those proposed in [20]. Where:

$$C_1 = C_2 = 0.5 + \log(2)$$
, and $w = 1/(2*\log(2))$ (3)

For more explanation of PSO algorithm, the general pseudo-code of PSO algorithm is as in Table 1.

Table (1): Pseudo-code of PSO algorithm

|] | Initialize the population's particles—including the searching positions and velocities—randomly. |
|---|---|
|] | Execute |
|] | For every particle. |
| (| Calculate the fitness value. |
| | Set current value as the new X_i^{PB} if the fitness value larger than the historically best X_i^{PB} |
|] | End |
|] | From all the particles, pick the one with the highest fitness value as X _{GB} . |
|] | For every particle |
|] | Determine the particle velocity for each one using Eq.1 |
| 1 | Update particle position according equation Eq. 2 |
|] | End |
|] | Repeat as necessary to reach the maximum iterations or the minimum error requirement |

In this work, we use PSO technique implemented offline to obtain optimal operating condition for maximize the product of the exothermic batch reactor type. As illustrated in the next sections, PSO is also performed online to maximize the performance of GMC for the batch reactor. (PSO is implemented offline: meaning PSO is run for the simulated model of the batch reactor where the process is offline). (PSO is performed online: meaning the PSO is attenuated the parameters of the controller GMC during the process is running with its nonlinear estimator). In the two steps, PSO is implemented using MATLAB© (Matlab 2020b) on Windows 10 using laptop Intel(R) Core (TM) i5-5300U CPU @ 2.30GHz 2.29 GHz.

3. NONLINEAR BATCH REACTOR MODEL

The benchmark batch process modeling used in this work was created by [14] and is presented in figure (2). The procedure appears to include a permanent, liquidphase, second-order, well-mixed exothermic reaction. The equivalent equations are listed below:

First reaction: $A + B \rightarrow C$ Second reaction: $A + C \rightarrow D$

The principal reaction, reaction 1, produces the desired product, C. The undesired product D is produced by reaction 2. The batch reactor's mass balance and energy balance make up the plant modeling.

3.1 Mass Balance

Mass balance of the raw materials MA and MB, also mass balance of desired and undesired products MC and MD, respectively, are as follow:

$$\frac{\mathrm{d}M_{\mathrm{A}}}{\mathrm{d}t} = -\mathrm{k}_{1}\mathrm{M}_{\mathrm{A}}\mathrm{M}_{\mathrm{B}} - \mathrm{k}_{2}\mathrm{M}_{\mathrm{A}}\mathrm{M}_{\mathrm{C}} \tag{4}$$

$$\frac{dM_B}{dt} = -k_1 M_A M_B \tag{5}$$

$$\frac{\mathrm{d}M_{\mathrm{C}}}{\mathrm{d}t} = \mathrm{k_1}\mathrm{M_A}\mathrm{M_B} - \mathrm{k_2}\mathrm{M_A}\mathrm{M_C} \tag{6}$$

$$\frac{\mathrm{d}M_{\mathrm{D}}}{\mathrm{d}t} = \mathrm{k_2}\mathrm{M_A}\mathrm{M_C} \tag{7}$$

The previous equations (4-7) can be rewrite as state space equation as follows:

$$\begin{bmatrix} \frac{dM_{A}}{dt} \\ \frac{dM_{B}}{dt} \\ \frac{dM_{C}}{dt} \\ \frac{dM_{D}}{dt} \end{bmatrix} = \begin{bmatrix} 0 & -k_{1}M_{A} & -k_{2}M_{A} & 0 \\ 0 & -k_{1}M_{A} & 0 & 0 \\ 0 & k_{1}M_{A} & -k_{2}M_{A} & 0 \\ 0 & 0 & k_{2}M_{A} & 0 \end{bmatrix} \begin{bmatrix} M_{A} \\ M_{B} \\ M_{C} \\ M_{D} \end{bmatrix}$$
(8)

$$k_1 = \exp\left(k_1^1 - \frac{k_1^2}{T_r + 273.5}\right)$$
, $k_2 = \exp\left(k_2^1 - \frac{k_2^2}{T_r + 273.5}\right)$ (9)

Where:

 M_A , M_B , M_C and M_D : Concentration of component (A, B, C and D respectively), kmol

 k_1 , k_2 : rate constant for reaction 1,2, respectively, kmol⁻¹ s⁻¹

- k₁¹, k₂¹: rate constant 1 for reaction 1,2, respectively
- k_1^2 , k_2^2 : rate constant 2 for reaction 1,2, respectively,
- T_r : Reaction Temperature (°C)

From equations (5-7), we can conclude that:

$$\frac{\mathrm{d}M_{\mathrm{B}}}{\mathrm{d}\,\mathrm{t}} + \frac{\mathrm{d}M_{\mathrm{c}}}{\mathrm{d}\,\mathrm{t}} + \frac{\mathrm{d}M_{\mathrm{D}}}{\mathrm{d}\mathrm{t}} = 0 \tag{10}$$

Hence:

 $M_{\rm D}(t) = M_{\rm D}(0) + M_{\rm c}(0) + M_{\rm B}(0) - M_{\rm B}(t) - M_{\rm c}(t)$ (11)

Where: $M_D(0)$, $M_c(0)$ and $M_B(0)$ are the initial conditions of concentration of substances (D, C and B respectively).

| M _A (0) :12 Kmol | k_1^1 : 20.9057 | U: 40.84kJ/min.m ² °C | C_{PA} ::75.31 kJ/(kmol°C) |
|-----------------------------|---------------------------------------|-------------------------------------|--------------------------------------|
| M _B (0): 12 Kmol | k ₁ ² : 10000 | A: 6.24 m ² | C_{PB} ::167.36 kJ/(kmol°C) |
| M _C (0): 0 Kmol | k ₂ ¹ : 38.9057 | ΔH ₁ : 41840.0 kJ kmol-1 | C _{PC} ::217.57 kJ/(kmol°C) |
| M _D (0):0 Kmol | k ₂ ² : 17 000 | ΔH ₂ : 25105.0 kJ kmol-1 | C_{PD} ::334.7 kJ/(kmol°C) |





Fig. (3): Batch Reactor is represented by Simulink and putting Tr equal the optimal value obtained (Trbest) by implemented PSO offline

3.2 Energy Balance

The energy balance around the reactor's contents is as follows, assuming that the heat transported throughout the system is larger than the heat retained in the reactor's walls [22]:

$$\frac{\mathrm{dT}_{\mathrm{r}}}{\mathrm{dt}} = \frac{\mathrm{Q}_{\mathrm{r}} + \mathrm{UA}(\mathrm{T}_{\mathrm{j}} - \mathrm{T}_{\mathrm{r}})}{\mathrm{W}_{\mathrm{r}}\mathrm{C}_{\mathrm{Pr}}}$$
(12)

$$Q_r = -\Delta H_1 R_1 - \Delta H_2 R_2 \tag{13}$$

$$W_r = M_A + M_B + M_C + M_D \tag{14}$$

$$C_{Pr} = \frac{C_{PA}M_{A} + C_{PB}M_{B} + C_{PC}M_{C} + C_{PD}M_{D}}{W_{r}}$$
(15)

$$R_1 = M_A M_B k_1$$
, $R_2 = M_A M_C k_2$ (16)

Where:

Tr: Reaction Temperature (°C), Tj: Jacket Temperature (°C), Qr: Heat Release by Reaction (K Joul/min)

Wr: Reactor Weight (kg), R_1 , R_2 : Reaction rate for reaction 1, 2 respectively (kmol/s).

U: heat-transfer coefficient of reactor (kW/ m 2 $^{\circ}C),$ A: area of the batch (m $^2)$

C_{Pr} : mass heat capacity of reactor contents (kJ/kg °C),

 C_{PA} , C_{PB}, C_{PC}, C_{PD} :molar heat capacity of component (A, B, C and D respectively) (kJ/kmol $^\circ C)$

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 $\Delta H_1, \Delta H_2$: heat of reaction for reaction 1,2 respectively (kJ/kmol). Table 2 describes the remaining constant parameters.

4. OPTIMAL OPERATING CONDITION DESIGN FOR BATCH REACTOR

The main important issue for the exothermic batch reactor is to know the best reaction temperature value which maximizes the desired product Mc. This optimization problem can be presented mathematically as follows:

$$\max_{T_r(t)} M_c \tag{17}$$

From mass balance equations (4&5) of the batch reactor, we observe the relation of the mass components MA, MB, MC and MD with the temperature reaction Tr. So, the optimization technique PSO is implemented by using MATLAB© and considering the mass balance equations (4&5).

There are constraints related to reactor safety, operational limits, and quality of the product. The temperature of the exothermic reactor should not exceed certain thresholds to avoid unwanted side reactions. So, the ideal reactor temperature in the range (20° C - 100° C). The operational batch time is not exceeded 2 hours. And the target to maximize the quantity of the product. So,

firstly the goal is to find the optimal operating condition that the ideal reactor temperature in the range ($20^{\circ}C - 100^{\circ}C$) to maximize the desired product Mc at the given batch time of 120min (2h) and with the initial charge of materials for the batch reactor described in Table 2.

The parameters of PSO are used as follows:

- *10 particles for each population
- *30 populations

Then we simulate the reactor process by using SIMULINK[©] in MATLAB[©] as shown in figure(3) to verify the obtained result through applying the best reactor temperature (Trbest).

5. Generic Model Control (GMC)

Although Generic Model Control (GMC) has been verified for many years, it is still used recently. The reason is that GMC is a model-based control approach that uses the process's non-linear model to determine control action. By combining two tuning settings, the required response can be obtained. GMC has a number of benefits for creating reactor controllers effectively [11]; such as the control algorithm directly uses the process model, GMC considers the nonlinear exothermic batch reactor without needing to its linearized model. Also GMC is simple to implement.

The GMC control algorithm is represented as:

$$\frac{dx}{dt} = K_1 (x_{sp} - x) + K_2 \int_0^t (x_{sp} - x) dt$$
(18)

Where x and x_{sp} represent the current and desired values of the control variable, respectively. As a result of a change in $\frac{dx}{dt}$, the process is brought back to steady state in the algorithm $K_1(x_{sp} - x)$. The second expression $K_2 \int_0^t (x_{sp} - x) dt$ is used to make the process have a zero offset.

5.1 GMC design for Batch Reactor

As shown in figure (2) that represents a schematic of the exothermic batch reactor type. In order to temperature control design for the exothermic batch reactor; the relationship between the control variable reactor temperature T_r and the manipulated variable T_j in the process model is needed. Equation (8) as mention above is giving this relation. Replacing x and x_{sp} with T_r and T_{rsp} in eq. (14), respectively, then by substituting of $\frac{dT_r}{dt}$ from eq. (14) in eq. (8). Thus the jacket temperature control T_j can be manipulated under GMC as follows:

$$T_{j} = T_{r} + \frac{W_{r}C_{Pr}}{UA} \left[K_{1} (T_{rsp} - T_{r}) + K_{2} \int_{0}^{t} (T_{rsp} - T_{r}) dt \right] - \frac{Qr}{UA}$$
(19)

Where K_1 and K_2 are tuning parameters of GMC; we choose them by using the implemented online PSO as will be described. $T_{rsp} = 92.4634$ °C is considered as obtained from the previous section (optimal operation condition). [14] converted the equation (15) to the discrete form as follows:

$$T_{j}(k) = T_{r}(k) + \frac{W_{r}C_{Pr}}{UA} \left[K_{1} \left(T_{rsp} - T_{r}(k) \right) + K_{2} \sum_{0}^{k} \left(T_{rsp} - T_{r}(k) \right) \Delta t \right] - \frac{Qr}{UA}$$
(20)

Where Δt is the sampling time (= 0.01 min). Also [14] used the following equation (17) to evaluate Tjsp(k) depending on Tj(k) from equation (16);

$$T_{jsp}(k) = T_j(k) + \frac{\tau_j}{\Delta t} [T_j(k) - T_j(k-1)]$$
 (21)

However, we evaluates step point jacket temperature Tjsp (k) from feedback reactor temperature Tr(k) then the jacket temperature Tj(k) is obtained from Tjsp (k). So we replaced Tj(k) byTjsp (k) in equation (16) to be:

$$T_{jsp}(k) = T_r(k) + \frac{W_r C_{Pr}}{UA} \left[K_1 \left(T_{rsp} - T_r(k) \right) + K_2 \sum_{0}^{k} \left(T_{rsp} - T_r(k) \right) \Delta t \right] - \frac{Qr}{UA}$$
(22)

Also in equation (17), we replace Tjsp(k) by Tj(k) and vice versa. So the equation is as follow:

$$T_{j}(k) = T_{jsp}(k) + \frac{\tau_{j}}{\Delta t} [T_{jsp}(k) - T_{jsp}(k-1)]$$
 (23)

5.2 Applying PSO online to design GMC for Batch Reactor

K1 and K2 parameters of GMC controller are manipulated online by using PSO according to cost function suggested that is the summation of Step Response Parameters (SRP). SRP equation is as follows:

$$SRP = \omega_0 \cdot tr + \omega_1 \cdot ts + \omega_2 \cdot M_p + \omega_3 \cdot E_{ss}$$
(24)

Where tr, ts, Mp and Ess are rise time, settling time, maximum overshoot and steady state errors, respectively. Considering ω_0 , ω_1 , ω_2 and ω_3 are equal 1.

The implemented PSO to manipulate K1 and K2 parameters of GMC to obtain best performance has the following parameters:

*10 particles for each population

*30 populations

The implemented PSO calls the Simulink file that represents the whole control system which consists of the plant, estimation of MA, MB and MC (as described in the next section), calculation of the heat- release Qr as in eq.(8) and GMC controller as shown in figure(4).

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Fig. (4): Total control system consists of the plant, the estimate and proposed on line manipulated GMC controller by implemented PSO online

6. STATE OBSERVER DESIGN

In reality, not all state components are accessible for feedback. Potential explanations include the lack of sensors, the cost of sensors, or the fact that the sensors that are available are unacceptable (due to high noise, high power consumption, etc.). State observers are used to estimate unmeasured state components. Given the output and control input measurements of the physical system, a state observer is a system that estimates the internal states of a real system [25].

In our Case, the reactor has 4 state variables (MA, MB, MC and MD) and control input (reactor Temperature Tr). We have to estimate the 4 state variables. Depending of the theoretical basics of nonlinear state observer design as described in [16], a nonlinear observer is designed to estimate online 3 state variables by measuring only one state variable which is the concentration of raw material A (MA). Also equation (4) which is a relation between derivative of three state variables MA, MB and MC is used to estimate the value of MD from equation (7).

Consider the batch reactor equations:

$$\frac{\mathrm{dx}}{\mathrm{dt}} = \mathrm{Ax} \tag{25}$$

$$y = Cx \tag{26}$$

Where
$$x = \begin{bmatrix} MA \\ MB \\ MC \end{bmatrix}$$
, $A = f(T_r, MA) = \begin{bmatrix} 0 & -k_1MA & -k_2MA \\ 0 & -k_1MA & 0 \\ 0 & k_1MA & -k_2MA \end{bmatrix}$, $C = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}$ and so $y = MA$

From equation (21), the matrix A is a function of a control input (temperature reaction Tr) which is obtained from the implemented controller GMC and the state MA which is the measured output of the state space equation (22). So, a state observer for this plant is designed relying on (Tr and MA measurements). This plant is completely observable (A, C) that is the main condition for designing the observer.

The state observer equation as follows:

$$\frac{d\hat{x}}{dt} = A\hat{x} + G(y - C\hat{x})$$
(27)

where \hat{x} is the three estimated state variables = [MAe MBe MCe] and G is the observer gain matrix. The observer gain matrix is chosen to assure the stability of the suggested controller batch reactor system as shown in the next section.

6.1 Stability Analysis and Robustness

Let
$$e = \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix} = x - \hat{x}$$
; hence.
$$\frac{de}{dt} = (A - GC)e$$
(28)

One choice of G = MA
$$\begin{bmatrix} l_1 \\ -k_1/\alpha \\ -k_2 \end{bmatrix}$$
, $l_1, \alpha > 0$;
 $\therefore A - GC = MA \begin{bmatrix} -l_1 & -k_1 & -k_2 \\ k_1/\alpha & -k_1 & 0 \\ k_2 & k_1 & -k_2 \end{bmatrix}$ (29)

Consider Lyapunov function:

$$V = e_1^2 + \alpha e_2^2 + e_3^2$$
(30)

$$\dot{V} = -2MAl_1e_1^2 - 2MAk_1\alpha e_2^2 - 2MAk_2e_3^2 + 2MAk_1e_2e_3 < 0$$
(31)

Provided that $\alpha > \frac{k_1}{4k_2}$, hence $e \rightarrow 0$ and $\hat{x} \rightarrow x$.

Consider the control Tj in eq. (19) with estimated heat release $\widehat{Q_r}$ and estimated reactor weight $\widehat{W_r}$ calculated using the estimated MAe, MBe, MCe, MDe (by neglecting variation in Cpr)

$$\therefore T_{j} = T_{r} + \frac{\widehat{W}_{r}C_{Pr}}{UA} \left[K_{1}(T_{rsp} - T_{r}) + K_{2} \int_{0}^{t} (T_{rsp} - T_{r}) dt \right] - \frac{\widehat{Q}r}{UA}$$
(32)

Where: $\widehat{W}_{r} = MAe + MBe + MCe + MDe$ and

$$\widehat{Q}r = -\Delta H_1 k_1 MAe MBe - \Delta H_2 k_2 MAe MCe$$

$$\therefore T_{j} = T_{r} + \frac{W_{r}C_{Pr}}{UA} \left[K_{1}(T_{rsp} - T_{r}) + K_{2} \int_{0}^{t} (T_{rsp} - T_{r}) dt \right] - \frac{Q_{r}}{UA} - \frac{\widetilde{W}_{r}C_{Pr}}{UA} \left[K_{1}(T_{rsp} - T_{r}) + K_{2} \int_{0}^{t} (T_{rsp} - T_{r}) dt \right] + K_{2} \int_{0}^{t} (T_{rsp} - T_{r}) dt \right] + \frac{\widetilde{Q}_{r}}{UA}$$
(33)

Sub. of Tj from eq. (33) in eq. (12):

Let $\widetilde{W}_{n} = W_{n} - \widehat{W}_{n} : \widetilde{\Omega}_{n} = \Omega_{n} - \widehat{\Omega}_{n}$

$$\therefore \frac{dT_r}{dt} = K_1 (T_{rsp} - T_r) + K_2 \int_0^t (T_{rsp} - T_r) dt - \frac{\widetilde{W}_r}{W_r} \Big[K_1 (T_{rsp} - T_r) + K_2 \int_0^t (T_{rsp} - T_r) dt \Big] + \frac{\widetilde{Q}_r}{W_r}$$
 (34)

From $\widetilde{W}_r, \widetilde{Q}_r \rightarrow 0$;

$$\therefore \frac{\mathrm{d}T_{\mathrm{r}}}{\mathrm{d}t} = \mathrm{K}_{1}(\mathrm{T}_{\mathrm{rsp}} - \mathrm{T}_{\mathrm{r}}) + \mathrm{K}_{2} \int_{0}^{t} (\mathrm{T}_{\mathrm{rsp}} - \mathrm{T}_{\mathrm{r}}) \mathrm{d}t \quad (\mathbf{35})$$

 $\begin{array}{ll} {\rm Or} & \frac{d^2 T_r}{dt^2} + K_1 \frac{d T_r}{dt} + K_2 T_r = \ K_2 T_{rsp} \\ {\rm Hence} \ T_r \to T_{rsp} \end{array}$

Therefore the observer gain G is designed to achieve the stability condition. Also we use S-function in Matlab R2020b to implement the batch reactor (eqs.25&27) and its estimated system as shown in Simulink figure (4). So, the whole control system consists of plant, estimation, the controller GMC and calculated Qr is implemented in Simulink[©] Matlab[®] R2020b as shown in figure (4).

It is crucial to evaluate the adaptability of the proposed GMC-based online PSO controller in terms of changes in operational and process parameters. The following changes are made to the process/operational parameters:

- a. $\Delta H_1 and \Delta H_2$ reaction temperatures are enhanced by 30% of their nominal value. For many reaction systems, the true value of the heat of reaction may not be available. As a result, this could be a source of process-model mismatch.
- b. To represent variations in operating circumstances induced by fouling of the heat exchanger (jacket) over time, the heat transfer coefficient (U) is reduced by 40% of its nominal value.
- c. The reactant initial charge (MA and MB) is lowered by 30%. This illustrates changes in operating conditions that could be caused by a shift in product demand, an accidental failure of the charging system, or design scale-up concerns.

7. SIMULATION RESULTS

- 7.1The result of the implemented PSO offline for obtain the optimal condition of the batch reactor gives the best reactor temperature at (Tr= 92.4634°C) and optimize the desired product at (Mc=6.5126). As shown in Figure (5) in the 10th iteration of the program achieves the target.
- 7.2Figure (6) depicts the raw materials (MA&MB), intended product MC, and waste product MD for the best reaction temperature (Tr) achieved. With applying the obtained best reactor temperature (Trbest) on the simulated batch reactor as shown in figure (3) (in section 4), figure (7) proves the symmetric result of the states MA, MB, MC and MD with figure (6).



Fig. (5): The result of Solving Optimization Problem by implemented PSO offline to obtain best Tr optimizes Mc



Fig. (6): The Schematics of MA, MB, MC and MD for the obtained best reaction Temperature Tr.



Fig. (7): describes the symmetric of the states MA, MB, MC and MD with figure (6) by using simulated batch reactor as described in Fig. 3

7.3 The implemented PSO online to manipulate the GMC for the batch reactor gives $K1=0.9 \text{ min}^{-1}$ and $K2=10^{-10} \text{ min}^{-1}$ that give best cost function SRP = 22.7613 with rise time =10.0321min, settling time =12.7292min, Maximum overshoot = 0 and steady state error = 7.8160*10⁻¹³. However by using reference [12] for

K1=0.2min⁻¹ and K2= 10^{-4} min⁻¹, the cost function gives SRP=31.2150with rise time =11.2282 min, settling time =19.7947min, Maximum overshoot = 0.0056 and steady state error = 0.1865. Figure 8 proves the improved performance for the controller GMC by using the suggested K1 and K2 over the reference in [12].



Fig. (8): Reaction temperature (Trbest) using implemented PSO online compared with the previous reference work (TrbestR).

7.4 By applying the observer design, the simulation results achieve the matching between the real and estimated states as shown in figure (9). The calculated heat release Qr is shown in figure 10. Figure 11 shows outputs of the proposed controller GMC that Temperature jacket step point Tjsp, temperature jacket Tj, reaction temperature Tr with respect to Temperature step point Trsp.



Fig. (9): Assuring the similarity of the estimated states (MAe, MBe, MCe and MDe) with the real states of the plant (MA, MB, MC and MD), respectively



Fig. (10): The calculated Heat Release Qr



- Fig. (11): Outputs of the proposed controller GMC; temperature jacket step point Tjsp, temperature jacket Tj, reaction temperature Tr w.r.t Temperature step point Trsp.
- 7.5 The robustness of the suggested controller, as seen in Figures (12–15), is demonstrated by the simulation results. Additionally, table (3) provides a detailed performance analysis of the suggested controller based on the robustness tests. Using Table 3 and earlier Figures, zero steady state.



Fig. (12): The Heat Release Qr calculated with increasing heat of reactions by 30% compared to ordinary Qr





Error and zero overshoot although the changes of the operational and process parameters with high rating assure the robustness of the proposed online PSO based on GMC.



Fig. (14): Response of the proposed Online PSO based on GMC with reducing the heat transfer coefficient (U) by 40%



Fig. (15): Response of the proposed Online PSO based on GMC with reducing the initial charges (MA and MB) by 30%

| | Rise Time(min) | SettlingTime(min) | Overshoot | Steady State Error |
|---|----------------|-------------------|-----------|--------------------|
| 1.(ΔH_1 and ΔH_2)are increased by 30% | 9.7737 | 12.6472 | 0.0 | 0.0 |
| 2. (U) is decreased by 40% | 15.8477 | 19.4369 | 0.0 | 0.0 |
| 3.MA(0)and MB(0) are reduced by 30% | 18.9595 | 23.1945 | 0.0 | 0.0 |

Table (3): Performance of the proposed controller according to the robustness tests

8 CONCLUSIONS

The aims of this work are achieved by implementing an effective, online, stable and robust generic model controller GMC based on PSO for control the nonlinear exothermic batch reactor type. Firstly, PSO is implemented to obtain set point reaction temperature that maximize the desired product of the exothermic batch reactor. Then the optimal nonlinear generic model control (GMC) parameters based on cost function that depends on the high performance are chosen by implemented PSO online. Basic addition, an online nonlinear state observer is created to estimate the main states of the batch reactor type. This designed observer has advantages such as; its selected gain assures the stability of the nonlinear batch reactor controller system by using Lyapunov stability. Also, it saves the cost by depending on just one concentration sensor and reaction temperature sensor. The simulation results demonstrate the practicality of the online state observer, which provides matches between the four states and their actual. Also, the output of the simulation demonstrates the effectiveness, superior performance and robustness of the entire suggested method of temperature control for the reference exothermic batch reactor type.

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