Genetic algorithm based PID optimization in batch process control

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Genetic Algorithm Based PID Optimization in Batch Process Control

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***Abstract* — The primary aim in batch process is to enhance the process operation in order to achieve high quality and purity product while minimising the production of undesired by-product. However, due to the difficulties to perform online measurement, batch process supervision is based on the direct measurable quantities, such as temperature. During the process, a large amount of exothermic heat is released when the reactants are mixed together. The exothermic behaviour causes the reaction to become unstable and consequently the quality and purity of the final product will be affected. Therefore, it is important to have a control scheme which is able to balance the needs of process safety with the product quality and purity. Since the chemical industries are still applying PI and PID to control the batch process, researchers are keen to optimize PID parameters using artificial intelligence (AI) techniques. However, most of these PID optimization techniques need online process model to predetermine the optimizer parameters. However in practice, the dynamic model of the batch process is poorly known. As a result, majority of the studies focused on acceptable performance instead of optimum performance of the batch process control. This paper proposes a new genetic algorithm (GA) optimizer which consists of additional information of the online estimated model parameters in addition to the PID parameters as the string of the GA. The simulation results show that the proposed GA auto-tuning method is a better candidate than the regular GA where the estimated model parameters in fitness function is capable to control the process temperature while avoiding model mismatch and disturbance condition.**

***Keywords* – process optimization; exothermic heat; temperature control; genetic algorithm**

I. INTRODUCTION

Chemical process operation mode can be classified into two categories: continuous and batch. Continuous process is usually used in large scale production lines, whereas batch process is used to manufacture small-volume products (e.g. pharmaceuticals, agrochemicals and etc). Batch process receives foremost attention due to its flexibility to adapt with variety products manufacturing. In general, batch process is aim to maximise the production of desired product while minimise the production of undesired by-product in a finite process duration. However, due to the difficulties to perform online measurement, batch process supervision is basically based on the direct measurable quantities, such as temperature [1].

Batch process control is proved to be a challenging task, especially exothermic reaction is involved since the dynamic behaviour of the process is highly nonlinear and varying with time [2]. If the heat released due to exothermic reaction exceeds the reactor cooling capacity, it will cause thermal runaway. As the result, it will affect the final product quality and will also pose safety issue to the plant. Thus, it is vital to control the process temperature in a desired trajectory.

Although many advanced control methods (e.g. generic model control [3], model predictive control [4], fuzzy logic [5] and etc) have been studied in the past, chemical industries are still implementing PI and PID controllers to control the batch process [6]. The main disadvantage of these methods is that the optimum results are seldom obtained due to the need of an experienced operator to manually tune the controller parameters. In order to reduce the dependency on human operator, artificial intelligence (AI) technique is proposed to auto-tune the PID parameters [7, 8, 9]. It can be concluded that most of these PID optimization techniques need to have process model to predetermine the optimizer parameters. Due to the dynamic model of the batch process is poorly known in practice, most of the studies only provide an acceptable performance instead of an optimum performance.

Hence, the purpose of this paper is to present a PID optimization technique using a newly design genetic algorithm (GA) to improve the batch operation performance. This proposed method with the additional information of the online estimated model parameters is able to adapt its fitness function and then evolve an optimum set of PID parameters to control the reactor temperature.

The organisation of this paper is described as follows. Section II describes the process modelling. Section III explains the proposed control technique. Section IV shows the results and discussions. Finally, Section V summarises the findings in this paper.

II. PROCESS MODELLING

The modelling of the batch process used in this research is based on the dynamic model proposed by Cott and

Macchietto [3], where a parallel and well-mixed liquid phase reaction is considered, as shown in (1) and (2).

Reaction 1: $A + B \rightarrow C$ (1)

Reaction 2: $A + C \rightarrow D$ (2)

Reaction 1 is the main reaction where reactant A and reactant B are mixed together and produce desired product C, whereas the Reaction 2 is the side reaction where reactant A reacts with the product C and produce undesired by-product D. Fig. 1 illustrates the batch reactor diagram.

A. Thermal Energy Balance

During the reaction process, liberated exothermic heat will further increase the reactor temperature. In order to maintain the reactor temperature in a desired trajectory, it should be cooled down using the surrounded jacket, as shown in Fig. 1. The change of reactor temperature can be formulated as (3).

$$\frac{dT_r}{dt} = \frac{(-\Delta H_1 R_1 - \Delta H_2 R_2) + UA(T_j - T_r)}{M_r C_{p_r}} \quad (3)$$

The change in the jacket temperature is mainly affected by the thermal energy difference between jacket and coolant, plus thermal energy difference between jacket and reactor, as shown in (4). The thermal energy will transfer from the hotter places to heat up the colder places.

$$\frac{dT_j}{dt} = \frac{F_j \rho_j C_{p_j}(T_c - T_j) - UA(T_j - T_r)}{V_j \rho_j C_{p_j}} \quad (4)$$

Initially, the reactor, jacket and coolant temperature are assumed to be equal as room temperature 20 °C. The range of jacket temperature and coolant temperature are assumed to be in the range of 20 °C to 120 °C due to the constraint of heat exchanger capacity.

B. Mass Balance

The reaction rate constants for k_1 and k_2 are highly depending on the reactor temperature through the Arrhenius equation, as shown in (5) and (6) respectively.

$$k_1 = \exp(k_1^1 - \frac{k_1^2}{T_r + 273.15}) \quad (5)$$

$$k_2 = \exp(k_2^1 - \frac{k_2^2}{T_r + 273.15}) \quad (6)$$

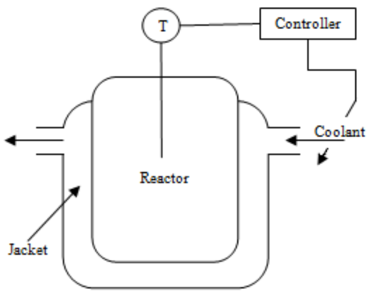


Figure 1. Batch reactor diagram

The reaction rates for Reaction 1 and Reaction 2 are depending on the reactants concentration and reaction rate constant, as described in (7) and (8) respectively.

$$R_1 = k_1 M_A M_B \quad (7)$$

$$R_2 = k_2 M_A M_C \quad (8)$$

The concentration of substance A, B, C and D are changed according to the reaction rate of (7) and (8) for Reaction 1 and Reaction 2, as shown from (9) to (12) respectively. The initial concentration of substance A, B, C and D are assumed to be 12 kmol, 12 kmol, 0 kmol and 0 kmol respectively.

$$\frac{dM_A}{dt} = -R_1 - R_2 \quad (9)$$

$$\frac{dM_B}{dt} = -R_1 \quad (10)$$

$$\frac{dM_C}{dt} = R_1 - R_2 \quad (11)$$

$$\frac{dM_D}{dt} = R_2 \quad (12)$$

C. Physical Parameters

The total charging molar inside the reactor and their total molar heat capacity are described in (13) and (14).

$$M_r = M_A + M_B + M_C + M_D \quad (13)$$

$$C_{p_r} = C_{p_A} M_A + C_{p_B} M_B + C_{p_C} M_C + C_{p_D} M_D \quad (14)$$

III. Control Technique

This study presumes that the process plant indicates the real experiment, in which all the parameters and their relationships are unknown in the controller. The modelling equations shown in Section II are mainly used to generate results to indicate the real experimental data, and the parameters are shown in Table I.

The proposed technique consists of two components: optimization scheme and controller. In the optimization scheme, genetic algorithm (GA) is proposed as the optimizer of PID controller parameters. This optimization method is able to adapt its fitness function depending on the dynamic changes in the reactor, and then evolving the optimum PID controller parameters.

On the other hand, PID is employed as the controller in this paper because it is still commonly applied in industries. It will determine the suitable coolant temperature based on the deviation between the optimal temperature profile and the current reactor temperature using the well-tuned parameters based on the proposed GA optimizer.

A. Optimization Scheme

The framework of the proposed GA is shown in Fig. 2. First, an initial population of solutions is randomly generated with a population size of 50. The output of this proposed GA function is the estimated relationship between the coolant temperature and the reactor

TABLE I.
MODELLING PARAMETERS AND DESCRIPTION

Parameter	Value	Unit	Description
A	6.24	m^2	Conduction surface between jacket and reactor
C_{pA}	75.31	kJ $kmol^{-1}$ °C^{-1}	Molar heat capacity of substance A
C_{pB}	167.36	kJ $kmol^{-1}$ °C^{-1}	Molar heat capacity of substance B
C_{pC}	217.57	kJ $kmol^{-1}$ °C^{-1}	Molar heat capacity of substance C
C_{pD}	334.73	kJ $kmol^{-1}$ °C^{-1}	Molar heat capacity of substance D
C_{pj}	1.8828	kJ kg^{-1} °C^{-1}	Heat capacity of coolant
C_{pr}	Refer to (14)	kJ $kmol^{-1}$ °C^{-1}	Total molar heat capacity
F_j	0.0058	m^3 s^{-1}	Flow rate of coolant into jacket
ΔH_1	-41840	kJ $kmol^{-1}$	Enthalpy change of Reaction 1
ΔH_2	-25105	kJ $kmol^{-1}$	Enthalpy change of Reaction 2
k_1^1	20.9057	-	Constant
k_1^2	10000	°C	Constant
k_2^1	38.9057	-	Constant
k_2^2	17000	°C	Constant
MWA	30	kg $kmol^{-1}$	Molar weight of substance A
MWB	100	kg $kmol^{-1}$	Molar weight of substance B
MWC	130	kg $kmol^{-1}$	Molar weight of substance C
MWD	160	kg $kmol^{-1}$	Molar weight of substance D
ρ	1000	kg m^{-3}	Total substance density
ρ_j	1000	kg m^{-3}	Coolant density
r	0.5	m	Radius of reactor
R_1	Refer to (7)	kmol min^{-1}	Reaction rate of Reaction1
R_2	Refer to (8)	kmol min^{-1}	Reaction rate of Reaction 2
T_c	-	°C	Coolant temperature
T_j	-	°C	Jacket temperature
T_r	-	°C	Reactor temperature
T_{ref}	95	°C	Reference temperature
U	0.6807	kW m^{-2} °C^{-1}	Heat transfer coefficient
V_j	0.6912	m^3	Volume of jacket

temperature, and the PID parameters. The solutions of proposed GA are strings of five parameters, which is able to characterise all the process input-output relationships and PID parameters, as shown in Fig. 3.

The fitness of each solution is calculated using the estimated process relationship. The best solution obtains highest fitness value; otherwise, it will obtain lower fitness value. The equation of fitness function is described in (15) and (16).

$$T_{est} = M \times T_c + C \tag{15}$$

$$Fitness = \frac{1}{(T_r - T_{est})^2} + \frac{1}{(T_{ref} - T_{est})^2} \tag{16}$$

where T_{ref}, T_r, T_{est} and T_c are the reference temperature, reactor temperature, estimated reactor temperature and coolant temperature respectively. M and C are developed based on the relationship between coolant temperature and reactor temperature. The first term of (16) is used to obtain the best estimation of process input-output relationship, whereas the second term is used to determine the optimum PID parameters in the string. The process input-output relationship is used to calculate the fitness of each PID parameters set.

Ranking method is used in selection operation. This operation emphasises the fittest solution in the population by duplicating those solutions in the mating pool and hoping that their offspring will in turn have even higher fitness value while maintaining the population size.

In crossover operation, blending method is used with a rate of 0.9. This operation will randomly pick up two solutions, called parent, from the mating pool. Some portions from both parents will be exchanged and create two new solutions, called offspring. This method combines variable values from both parents into new variable values in the offspring. The first offspring variable value comes from a combination of two corresponding parent variable values, whereas the second offspring is merely the complement of the first offspring, as described in (17) and (18).

$$x_{n1} = \beta \cdot x_{p1} + (1-\beta) \cdot x_{p2} \tag{17}$$

$$x_{n2} = \beta \cdot x_{p2} + (1-\beta) \cdot x_{p1} \tag{18}$$

where x_n is the offspring, x_p is the parent, β is a random number, which is in between 0 and 1.

The mutation operator helps in randomly searching other areas of the solution space that may be unexplored and might be containing the global maxima. However, the probability of mutation must be low in order to prevent the loss of fit solutions and affect the convergence of the solutions. Hence, the mutation rate in this paper is set as 0.01.

The stopping criterion of the GA is whenever the maximum number of generation is reached. In this work, the maximum number of generation is set to 20. Hence, the GA will stop after 20 generations and choose the optimum PID parameters.

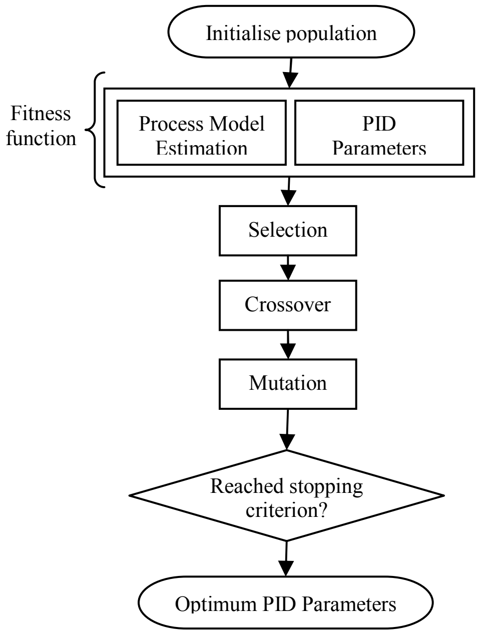


Figure 2. Framework of proposed GA

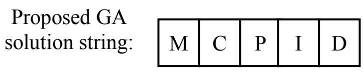


Figure 3. Proposed GA solution string

B. Controller

The controller model is based on PID control algorithm, as described in (19).

$$u(t) = K_p e(t) + K_i \int_0^t e(\tau) d\tau + K_d \frac{de(t)}{dt} \qquad (19)$$

where $u(t)$ is the control variable, $e(t)$ is the error, K_p is the proportional parameter, K_i is the integral parameter, and K_d is the derivative parameter.

IV. Results and Discussion

This compares the performances of three types of controller: classical PID controller, regular GA-PID controller and the proposed GA-PID controller with additional parameters at the fitness function.

First of all, PID parameters are manually tuned using all the nominal process parameters and Fig. 4(a) illustrates its performance. It can be observed that the PID controller performs well in the nominal case if the PID parameters are well-tuned subjected to the nominal condition. The reactor temperature is raised to the desired temperature set point in 20 min. Fig. 4(b) shows the liberated exothermic heat during the process.

However, it is very important to test the robustness of the controller with unpredictable faults and disturbances because the reactor must always be operated in safe condition in regardless of any faults. Therefore, PID controller with the well-tuned parameters in nominal case is tested under two aspects: model mismatch and external disturbance. The robustness of PID is then compared with the regular GA-PID and proposed GA-PID.

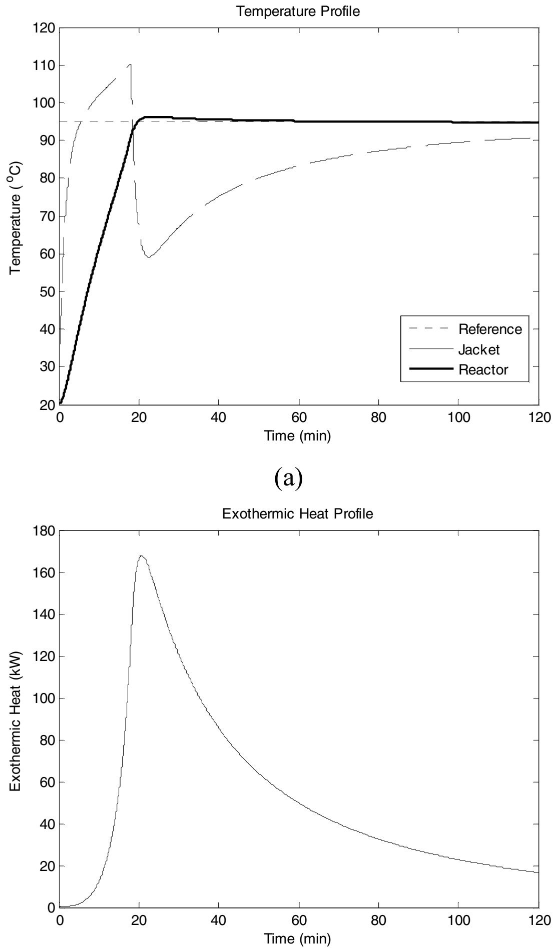
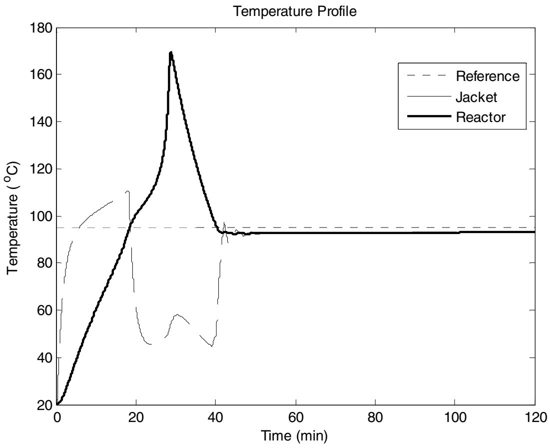


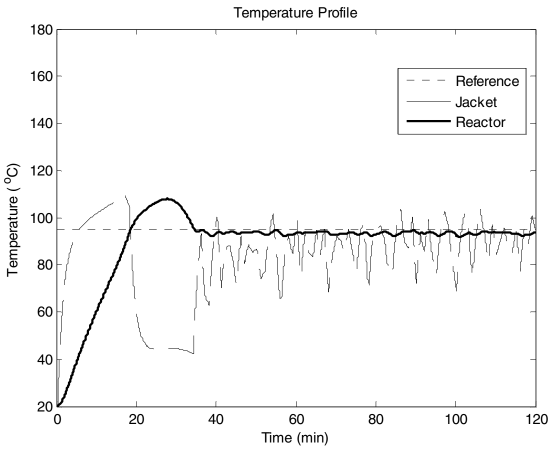
Figure 4. (a) PID performance, (b) exothermic heat profile under nominal case

The first robustness test involves 30 % and 10 % increment from the nominal value in reaction rate 1 and reaction rate 2 respectively. This test represents the presence of unmodelled reactions because the dynamic model of batch process is poorly known in practice. In reality, inherent variable time delay is one of the main challenges for the process controller to react efficiently [10]. Therefore, random time delay is introduced at the controller output due to the valve delay occurred in the jacket inlet stream. The performances of the controllers are shown in Fig. 5.

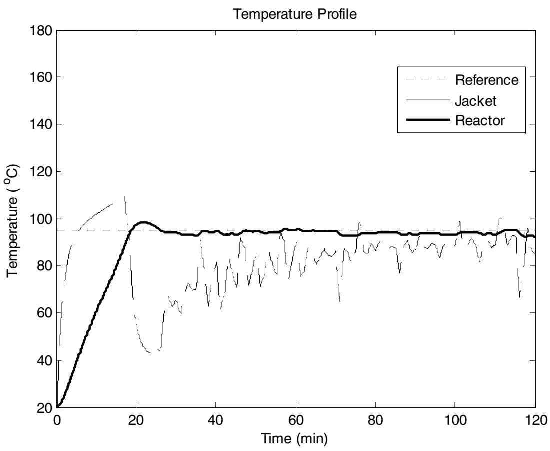
The simulation result shown in Fig. 5(a) illustrates that the PID controller has largest overshoot in the reactor temperature. This result shows that a preset PID controller is not robust in handling model mismatch condition. Therefore, AI technique is recommended to auto-tune the PID parameters. Fig. 5(b) demonstrates that the regular GA-PID with predetermined model parameters has an acceptable performance, whereas Fig. 5(c) shows that the proposed GA-PID has the best performance since it has the smallest overshoot in the reactor temperature. This is because by employing additional information of online estimated model parameters in the fitness function in GA, GA will adapt its fitness function parameters according to the environment changes and then able to evolve optimum PID parameters using the more accurate and updated information.



(a)

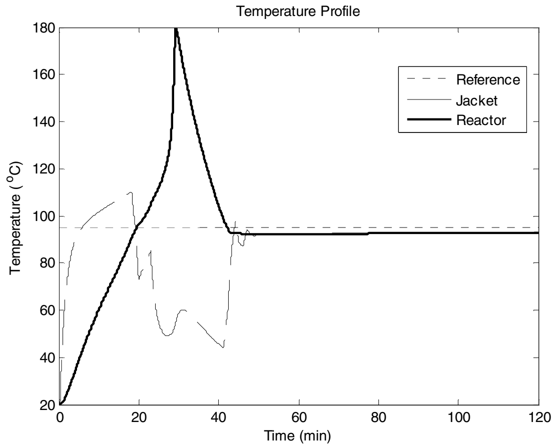


(b)

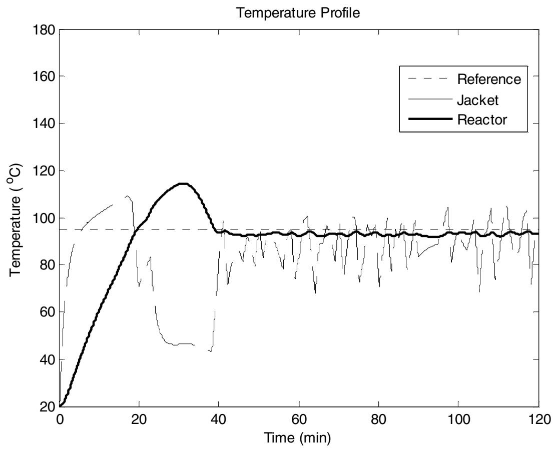


(c)

Figure 5. (a) Performance of PID, (b) Performance of regular GA-PID, (c) Performance of proposed GA-PID under model mismatch condition



(a)



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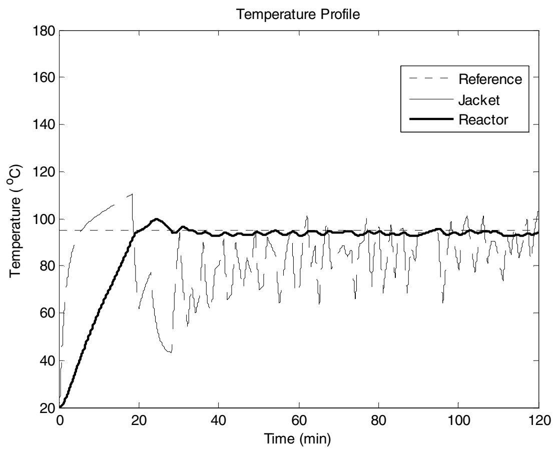
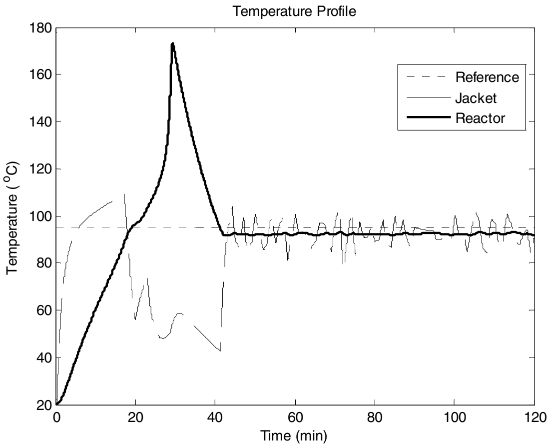


(c)

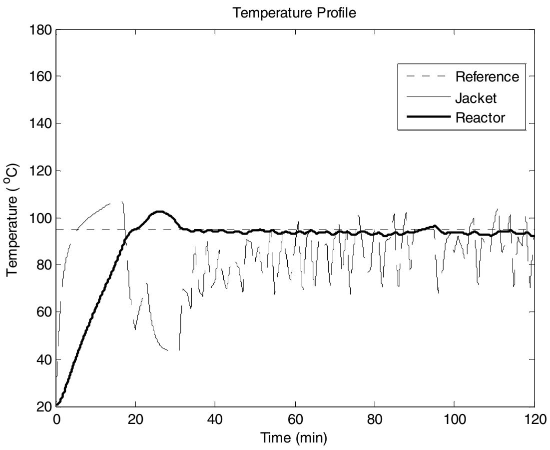
Figure 6. (a) Performance of PID, (b) Performance of regular GA-PID, (c) Performance of proposed GA-PID under external disturbance

The second robustness test involves a sudden shut down of the valve in jacket inlet stream at time 20 min to 23 min, and 90 min to 95 min. This test represents a short period of malfunction in the valve relay. Random time delay is also introduced in this robustness. The performances of the controllers are shown in Fig. 6.

As a result of disturbance rejection ability, Fig. 6 shows that the PID has worst performance, whereas the proposed control technique has the best performance in controlling the temperature when the external disturbance is introduced. Fig. 7 shows the performances of the regular GA-PID and the proposed GA-PID in dealing with the combination of model mismatch and external disturbance situations. Simulation is conducted to test the effectiveness of both controllers in a critical condition.



(a)



(b)

Figure 7. (a) Performance of regular GA-PID, (b) Performance of proposed GA-PID under combination case of model mismatch and external disturbance

The vigorous parameters changes force the process towards instability. Regular GA-PID with predetermined model in fitness function is not able to prevent the temperature runaway effectively, as shown in Fig 7(a). On the other hand, proposed GA-PID shows a less overshoot in the reactor temperature before the desired temperature is attained, as shown in Fig 7(b).

V. Conclusion

In this study, an exothermic process model with online estimated model parameters with the GA optimization scheme of PID controller has been developed based on the characteristic of the batch process. The proposed control technique consists of two components: optimization scheme and controller. The proposed GA optimizer is used to adapt its fitness function parameters and then optimize the PID parameters, whereas PID controller is used to control the reactor temperature by controlling the coolant temperature. From the simulation results, it can be verified that the proposed control method provides a more effective solution in temperature control due to its robustness against the variable time delay, model mismatch and external disturbance situations compared to the regular GA-PID with predetermined model parameter and non adaptive PID controller. In future, the proposed GA can be used to optimize the coolant flow rate as well as controlling the reactor temperature as a MIMO system.

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