

Control of Exothermic Batch Process using Multivariable Genetic Algorithm

Min Keng Tan, Helen Sin Ee Chuo, Yan Yan Farm, Heng Jin Tham, Kenneth Tze Kin Teo
 Modelling, Simulation & Computing Laboratory, Material & Mineral Research Unit
 School of Engineering and Information Technology
 Universiti Malaysia Sabah
 Kota Kinabalu, Malaysia
 msclab@ums.edu.my, hjtham@ums.edu.my, ktkteo@ieee.org

Abstract—The aim of this research is to control the reactor temperature of an exothermic batch process. During the process, large amount of heat will be released rapidly when the reactants are mixed together. The exothermic behaviour causes the reaction to become unstable and consequently poses safety concern to the plant personnel. In practice, heat is needed to speed up the reaction rate so that the overall process cycle time can be reduced whereas the cooling is employed to cool down the reactor in order to reduce excessive heat. Hence, this paper proposes genetic algorithm (GA) to control the process temperature with a predetermined temperature profile. GA exploits the probabilistic search method to optimise the specific objective function based on the evolutionary principle. Simulation assessment of the GA has been carried out using a benchmark exothermic batch process model. The results show that GA is able to control the reactor temperature effectively.

Keywords-exothermic batch process; genetic algorithm; multivariable control

I. INTRODUCTION

Batch process has received foremost concentration over the recent years due to its flexibility to adapt in various small volume productions of high-value added products, e.g. pharmaceuticals, polymers, and specialty chemicals [1, 2]. For the batch process, the raw materials (reactants) are initially charged into a reactor for a certain period to transform to another type of substance (product). In exothermic batch process, the environmental parameters of the reactor (e.g. pressure and temperature) need to be controlled in order to obtain the specific product quality and quantity. The process will be repeated after the previous batch completed.

From the industrial perspective, the main objective of the process is to minimise the batch cycle time to increase the profit. Hence, a fully heating up process is employed at the beginning of the process to speed up the reaction rate. However, a large amount of heat will be released rapidly as the process is being heated up. This continuous increasing temperature will cause the reaction to become unstable and will lead to thermal runaway if the generated heat exceeds the cooling capacity of the plant [3, 4]. As a result, the runaway reaction will pose a significant safety risk to the plant personnel as well as the equipment [5]. According to the report of U.S. Department of Energy in year 1996, chemical process hazard associated with the exothermic reaction is usually related to the process operation factors, such as operating temperature, concentration and flow rate which are deviated from the normal circumstance. Therefore, developing a suitable control strategy to control the batch process temperature is vital in order to avoid thermal runaway.

Nowadays, dual-mode controller (DMC) is still widely implemented in industries to control the reactor temperature due to its simplicity [6, 7]. In general, the control action of DMC can be divided into two stages. In the first stage, the DMC behaves as an open-loop system. A course of control actions is preset until the reactor temperature reaches a predetermined temperature. In the second stage, the conventional proportional-integral-derivative controller (PID) is used to maintain the reactor temperature at the desired trajectory. However, this method only performs in a limited range of operating conditions in which it is tuned since the DMC is practiced in an open-loop manner at the beginning stage. Besides, the parameters of PID are tuned by an operator based on his experience. Regrettably, a consistent performance is difficult to be obtained. Therefore, artificial intelligence techniques are introduced to control the process temperature.

Genetic algorithm (GA) is a stochastic global search method that mimics the evolutionary process [8, 9, 10]. GA associates its optimality concept through chosen objective function, yielding optimal solution with respect to such function. In the literatures, GA is proved to be effective in finding optimal solutions for various nonlinear problems, such as in traffic control, robotics, and power systems [11, 12]. In this work, GA is proposed to act directly as the controller to control the batch reactor temperature by manipulating the heater and coolant flow rate in order to maintain the reactor temperature into the desired trajectory. A benchmark exothermic batch process model is used to assess the performance of the proposed GA. This paper is organised as follows: Section II describes the mathematical modelling of the exothermic batch process, Section III discusses the genetic algorithm, Section IV explains the

simulation procedures. The performance of GA will be discussed in Section V and finally, Section VI summarises the findings of this paper.

II. MODELLING OF BATCH REACTION

A benchmark batch process modelling proposed by Cott and Macchietto [13] is used in this work. It is assumed that a second-order, well-mixed, and irreversible liquid-phase exothermic reaction occurs in the process. The stoichiometric equations are given in below.



Reaction 1 is the main reaction where reactant A and reactant B are mixed together and produce desired product C, whereas Reaction 2 is the side reaction where reactant A reacts with the product C and produce undesired by-product D. The plant modelling can be divided into three elements: reference temperature, mass balance, and thermal energy balance. Fig. 1 illustrates the batch process scheme. The heater is used to heat up the reactor contents in order to speed up the reaction rate, whereas the jacket is used to cool down the reactor temperature for avoiding the thermal runaway.

A. Reference Temperature

In the work of Cott and Macchietto [13], they found that the optimal isothermal reaction temperature is in the range of 90 °C to 100 °C. According to Kenneth *et al.* [14], they proposed that the reference temperature can be divided into two stages: rising stage and regulating stage. In the first stage, the reference temperature has to be increased at a specific rate from room temperature to the target temperature, whereas in the second stage, the final target temperature is perfectly regulated for a selected length of time. By considering both findings, this paper proposed that the reference temperature profile should be increased from 25 °C to 95 °C in the first 20 minutes, and then maintained at 95 °C until 120 minutes, as shown in Fig. 2.

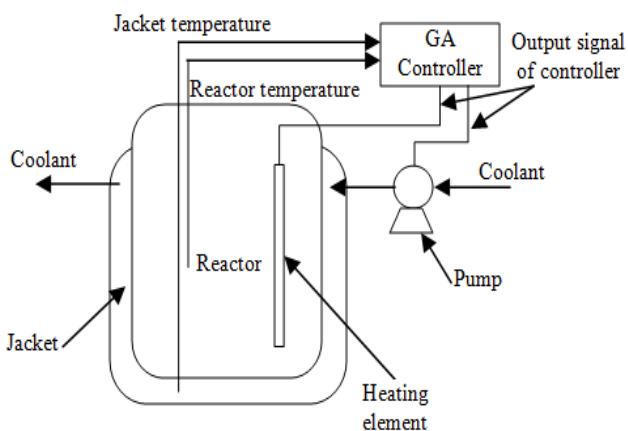


Figure 1. Batch process scheme.

B. Mass Balance

The law of conservation of mass is used to formulate the molar changes of all substances inside the batch reactor. This law stated that the amount of products produced by a chemical reaction is always equivalent to the amount of reactants consumed. Since both reactions are temperature dependence process, the reaction rate constant of both reactions can be modelled by using the Arrhenius equation, as shown in (1):

$$k_i = k_{0i} \exp\left(\frac{-E_{ai}}{k_B \cdot (T_r + 273.15)}\right), i = 1, 2 \quad (1)$$

where k_i is reaction rate constant for reaction i ; k_{0i} is pre-exponential factor for reaction i ; E_{ai} is activation energy for reaction i ; k_B is Boltzmann constant and T_r is reactor temperature.

The reaction rates for both reactions and production rates for the substances are described in (2) and (3) respectively. In the findings of [15], the initial charge that is equimolar in A and B will maximise the production of product C. Therefore, the initial concentrations of the reactant A, B, C, and D are assumed to be 12 kmol, 12 kmol, 0 kmol, and 0 kmol respectively.

$$\begin{bmatrix} R_1 \\ R_2 \end{bmatrix} = \begin{bmatrix} k_1 & k_2 \end{bmatrix} \cdot \begin{bmatrix} M_A & M_A \\ M_B & M_C \end{bmatrix} \quad (2)$$

$$\begin{bmatrix} \dot{M}_A \\ \dot{M}_B \\ \dot{M}_C \\ \dot{M}_D \end{bmatrix} = \begin{bmatrix} -1 & -1 \\ -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} R_1 \\ R_2 \end{bmatrix} \quad (3)$$

where R_i is reaction rate for reaction i ; and M_i is the concentration for substance i .

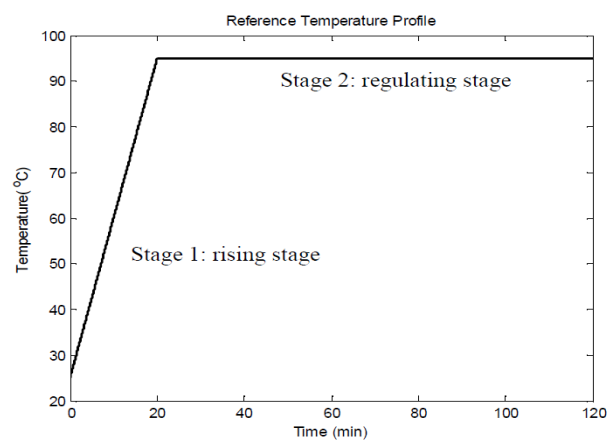


Figure 2. Reference temperature profile.

Other physical parameters of reaction, such as total weight of reactor contents, total molarity of reactor contents, and average molar heat capacity are shown in (4), (5) and (6) respectively.

$$W = \sum MW_i \cdot M_i, i = A, B, C, D \quad (4)$$

$$M_r = \sum M_i, i = A, B, C, D \quad (5)$$

$$C_{pr} = \frac{\sum (C_{pi} \cdot M_i)}{M_r}, i = A, B, C, D \quad (6)$$

where W is total weight of reactor substances; MW_i is molecular weight of substance i ; M_r is total number of mole of reactor substances; C_{pr} is average molar heat capacity; and C_{pi} is molar heat capacity of substance i .

C. Thermal Energy Balance

The reactor temperature is influenced by the heater, exothermic heat released, and the jacket temperature. The heater and the liberated heat will increase the reactor temperature, whereas the coolant flows into the jacket will cool down the reactor. In normal circumstance, the reactor temperature is usually higher than the jacket temperature. According to the energy conservation law, the total energy flow into the reactor is equal to the energy flow out from the reactor. Hence the energy balance of the process can be modelled as (7). The exothermic heat released is given in (8).

$$\begin{bmatrix} \dot{T}_r \\ \dot{T}_j \end{bmatrix} = \begin{bmatrix} \frac{1}{M_r C_{pr}} & 0 \\ 0 & \frac{(T_c - T_j)}{V_j} \end{bmatrix} \cdot \begin{bmatrix} Q_h \\ F_j \end{bmatrix} + \dots \quad (7)$$

$$\begin{bmatrix} 1 & -A_r(T_r - T_j) \\ \frac{1}{M_r C_{pr}} & \frac{M_r C_{pr}}{A_r(T_r - T_j)} \\ 0 & \frac{A_r(T_r - T_j)}{V_j \rho_j C_{pj}} \end{bmatrix} \cdot \begin{bmatrix} Q_r \\ U \end{bmatrix}$$

$$Q_r = \sum (-\Delta H_i \cdot R_i), i = 1, 2 \quad (8)$$

where T_r is reactor temperature; T_j is jacket temperature; T_c is coolant temperature; V_j is jacket volume; Q_h is heat released by heater; F_j is coolant flow rate; A_r is conducting area; ρ_j is coolant density; C_{pj} is mass heat capacity of coolant; Q_r is exothermic heat released; U is heat transfer coefficient between reactor and jacket; and ΔH_i is heat of reaction i . All the model parameters are shown in Table I.

TABLE I. PHYSICAL PROPERTIES AND PROCESS PARAMETERS

Parameter	Value	Unit	Parameter	Value	Unit
MW_A	30	kg / kmol	C_{pA}	75.31	kJ / (kmol °C)
MW_B	100	kg / kmol	C_{pB}	167.36	kJ / (kmol °C)
MW_C	130	kg / kmol	C_{pC}	217.57	kJ / (kmol °C)
MW_D	160	kg / kmol	C_{pD}	334.73	kJ / (kmol °C)
k_{01}	1.2×10^9	$\text{kmol}^{-1} \text{s}^{-1}$	E_{a1} / k_B	10000	K
k_{02}	7.9×10^{16}	$\text{kmol}^{-1} \text{s}^{-1}$	E_{a2} / k_B	17000	K
ρ	1000	kg / m ³	U	0.6807	kW / (m ² °C)
ρ_j	1000	kg / m ³	C_{pj}	1.8828	kJ / (kg °C)
V_j	0.6912	m ³	A	6.24	m ²
T_c	20	°C			

III. GENETIC ALGORITHM

GA is proposed to control the batch reactor temperature based on the biological evolution theory and Darwin's natural selection concept: "survival of the fittest". In this work, the proposed GA exploits heuristic search method to determine the suitable combination set of heater power and coolant flow rate profile in order to bring the reactor temperature to the desired path. In general, the mechanism of GA can be divided into three operators: selection, crossover and mutation. The framework of the proposed GA is shown in Fig. 3, and the detailed anatomy of each operator is discussed as follows:

A. Initialisation

In the beginning stage of GA, potential solutions are randomly generated and encoded into a string called chromosome. Since the GA is proposed to manipulate the heater power and coolant flow rate, the chromosome of the GA should consist of two genes. The first gene carries the information of the heater power, whereas the last gene encodes the coolant flow rate detail. Real-number chromosome representation method is applied in this work because the computing time of this method is faster than the binary chromosome representation method. From the simulation studies, the heater power is bounded in the range of 0 kW to 300 kW, whereas the coolant flow rate is bounded from 0 liter/s to 1 liter/s. After a few times of testing, it is found that the 50 population size of GA is sufficient for this work.

B. Fitness Function

The fitness evaluation function interprets the chromosomes in terms of physical representations and evaluates its fitness value based on the desired objective function (maintain the reactor temperature at desired path). This is an important step in the algorithm because GA evaluates the suitability of the solutions based on this function. In this work, the fitness of each solution can be calculated by taking the reciprocal of the absolute error, as

shown in (9). Those fitter chromosomes receive higher fitness value and will have preferential treatment in the reproduction process.

$$J = \frac{1}{|(T_{ref} - T_r)|} \tag{9}$$

where J is the fitness value of each chromosome; and T_{ref} is the reference temperature.

C. Selection

The primary aim of the selection operator is to put emphasis on the fitter chromosomes by duplicating those chromosomes to increase their offspring’s chance to have higher fitness value, and eliminate those unfit chromosomes while maintaining the population size. Ranking selection is used in this study because the best chromosomes have higher ranking and duplicate more when being selected in mating pool.

Firstly, all the chromosomes are sorted according to their fitness, ranked from least fit to the fittest. The fittest chromosomes assigned with higher weightage. The cumulative fitness is the summation of the ranks of chromosome in each generation. Then, the selection probability is generated by multiplying the total cumulative fitness with 50 random generated numbers. If the probability is within the cumulative fitness range of each individual, then the chromosome will be selected into the mating pool. In this operation, the fittest chromosome will have larger range of cumulative fitness and hence it will have higher probability of being selected from the mating pool.

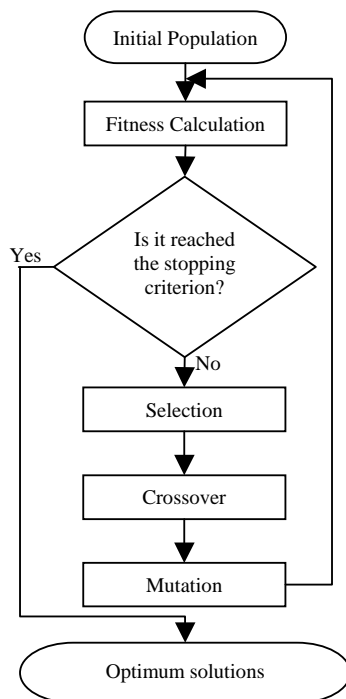


Figure 3. Framework of genetic algorithm.

D. Crossover

This operation is used to generate the new generation. In this operation, two chromosomes (called parents) are randomly picked up from the mating pool. Then, portions of the parents will exchange between each other and create another two new chromosomes (called offspring). Blending method is used to combine variable values from the two parents into new variable values in the first offspring, whereas the second offspring is merely the complement of the first offspring. The functions used to create new offspring are shown in (10) and (11).

$$x_{o1} = \beta \cdot x_{p1} + (1 - \beta) \cdot x_{p2} \tag{10}$$

$$x_{o2} = (1 - \beta) \cdot x_{p2} + (\beta) \cdot x_{p1} \tag{11}$$

where x_{oi} is offspring i ; x_{pi} is parent i ; and β is random number.

In order to preserve some fit solutions selected during the selection operator, the crossover probability is chosen as 0.9. It means only 90% of chromosomes are used in the crossover operation and 10% of the chromosomes are copied to the new generation.

E. Mutation

The mutation operator helps to prevent the search being trapped at local maxima. However, the mutation probability should be kept low to prevent the loss of too many fit chromosomes and affect the convergence. Therefore, the mutation rate is set to 0.01 in this case. This paper uses random mutation to randomly choose an individual from the new generation to be mutated.

F. Termination

The evolutionary process will be stopped when the number of generation reaches 10. When the evolutionary process is terminated, the majority chromosomes in the population are assumed to be the most suitable solution for the instantaneous condition. The parameters of the developed GA is summarised in Table II.

TABLE II. PARAMETERS OF THE DEVELOPED GA

Simulation Techniques:			
<i>Chromosome representation technique</i>		Real-number chromosome	
<i>Selection technique</i>		Rank selection	
<i>Crossover technique</i>		Arithmetic (blending) method	
Parameters:			
<i>Population size</i>	50	<i>Termination criteria</i>	10 generations
<i>Crossover probability</i>	0.9	<i>Mutation probability</i>	0.01

IV. SIMULATION

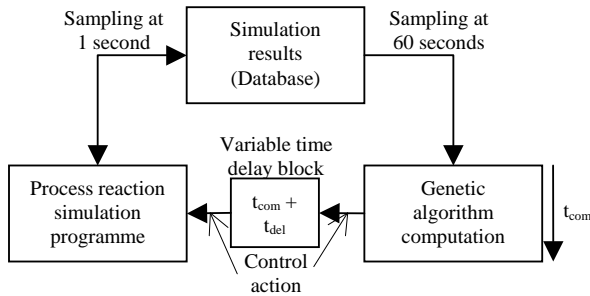
The modelling equations of the plant are developed in MATLAB. The batch process is simulated to obtain the relevant process measurement for every second, whereas the GA algorithm is sampled at the rate of 60 second. A stopwatch timer is used in MATLAB to measure the computational time delay of the proposed GA. Besides the computational time delay, the actuation time delay is considered and introduced into the simulation. The actuation time delay used in this paper is bounded in the range of 20 seconds to 30 seconds. The flowchart of simulation is shown in Fig. 4.

The robustness of the proposed GA is tested by two cases: measurement noise and model mismatch. Measurement errors are always present in the practical due to the sensor accuracy and precision. This situation is included in this work by adding noises to all the simulated temperature measurements. Reference [12] had introduced a first order moving average noise model equation to explain this condition, as shown in (12).

$$T_i = T_i + a^{(k)} - 0.866a^{(k-1)}, i = r, j, c \quad (12)$$

where $a(k)$ is normally distributed at k^{th} time interval; and T_i' is temperature after addition of measurement noise.

As stated in [16], it is vital to have a control strategy which is sensitive to the reaction variation. Therefore, R_1 is increased to 1.3 times from the original rate. This internal process parameter changes is also equivalent to the presence of unmodelled reactions. Table III indicates case studies used in this work.



- Note:
- 1) t_{com} is the computational time of genetic algorithm
 - 2) t_{del} is the actuation time delay

Figure 4. Simulation flowchart.

TABLE III. CASE STUDIES

Case	Description
I	Measurement noise + time delay
II	Model mismatch condition + time delay

V. RESULTS AND DISCUSSIONS

The exothermic heat released is shown in Fig. 5. The performance of the proposed GA in handling the measurement noise is shown in Fig. 6, whereas the Fig. 7 shows the performance of the proposed GA in handling the model mismatch condition.

From the Fig. 6(c) and Fig. 7(c), it can be seen that the GA attempts to provide full heating to heat up the reactant at the beginning of the process (first 20 min). As discussed in Section I, this step is important because it can reduce the overall batch cycle time. In order to avoid the reactor temperature deviates from the reference path, the coolant flow rate is manipulated to cool down the reactor if it is overshoot from the reference path. However, the coolant flow rate is kept as low as possible so that it will not affect the desired product reaction rate.

The exothermic heat released rate increases (shown in Fig. 5) as the reactor temperature increases (shown in Fig. 6(a) and Fig. 7(a)). Since the exothermic heat is released rapidly, the GA attempts to provide full cooling to the reactor. In this stage, the heater power will be automatically tuned to low whereas the coolant flow rate is kept high. Since the overshoot shown in Fig. 6(a) is shorter than the Fig. 7(a), the cooling period of the Case I is much shorter compared to the cooling period of the Case II. The undershoot occurred at $t = 25$ min shown in Fig. 6(a) causes the GA to stop the coolant flow rate and turn on the heater power to retrieve the reactor temperature back to the desired trajectory.

Since the GA evaluates the potential chromosomes based on the imprecise model in Case II (model mismatch condition), it causes GA delays in cooling down the reactor temperature and hence lead to the overshoot (around 5 %). From the Fig. 7(b) and Fig. 7(c), it can be observed that GA attempts to initiate full cooling (highest coolant flow rate) and low heating during $t = 20$ min to $t = 33$ min to reduce the reactor temperature to the desired trajectory.

Once the reactor temperature is closed to the desired path (for both cases), the GA will manipulate the heater power and coolant flow rate concurrently for keeping the reactor temperature at the desired trajectory.

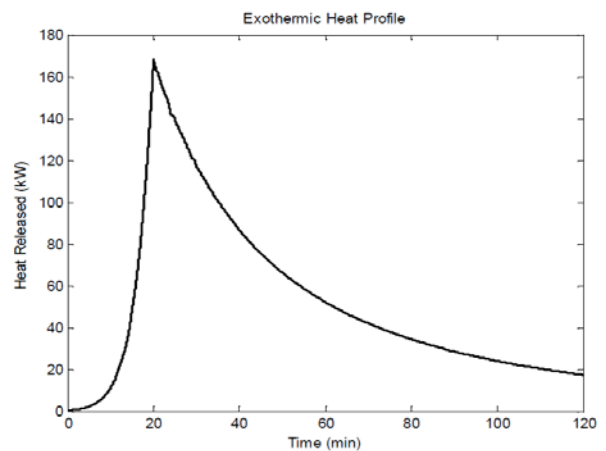


Figure 5. Exothermic heat released.

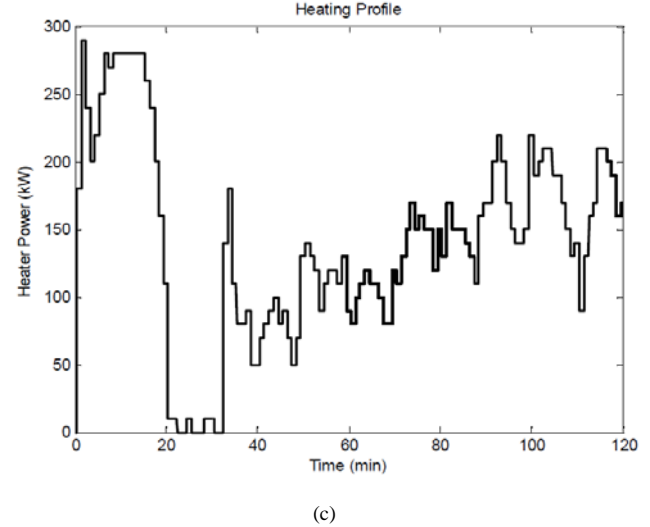
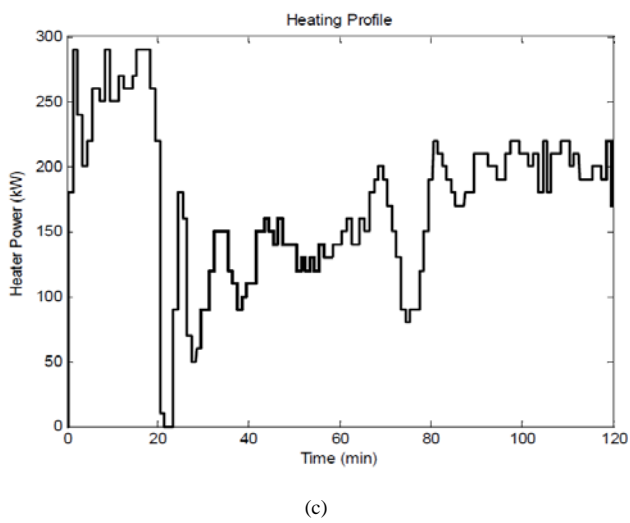
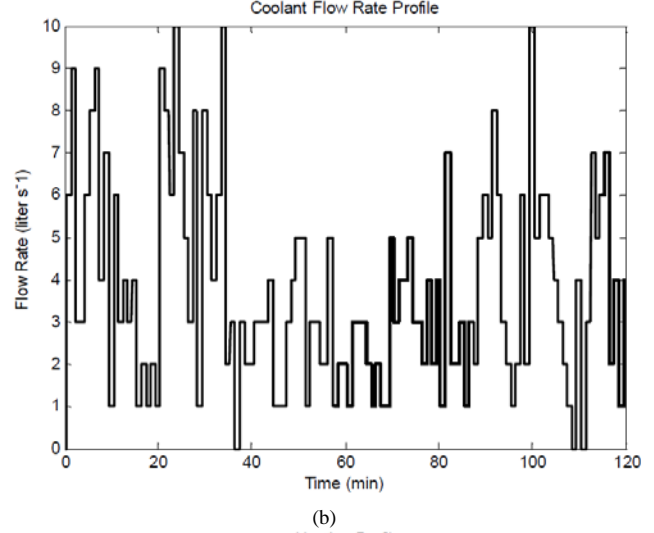
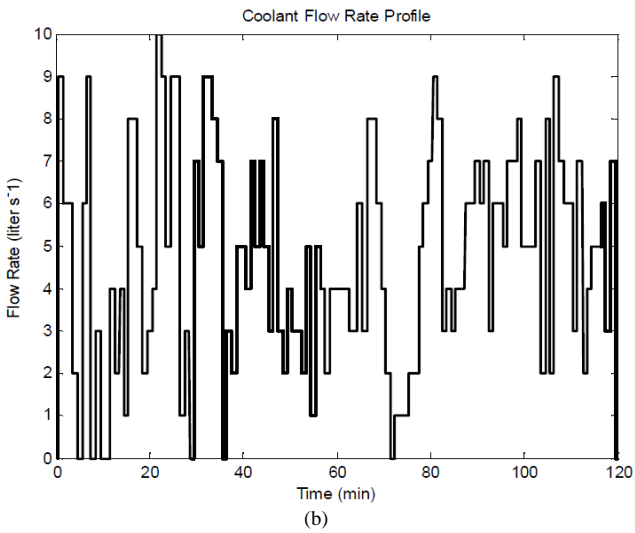
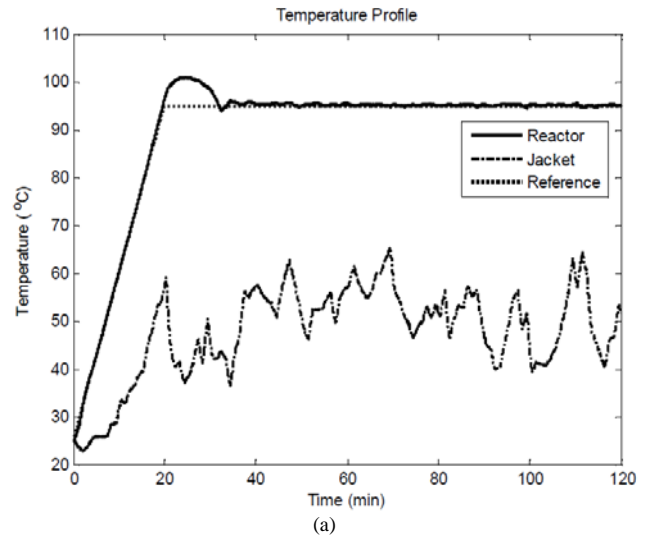
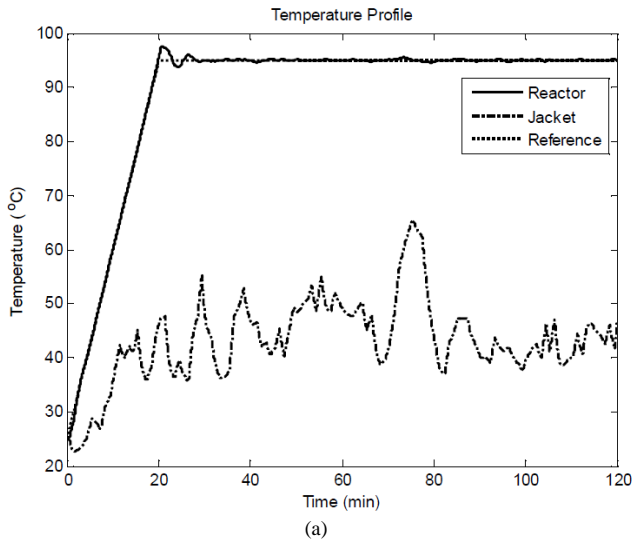


Figure 6. Performance of GA in handling measurement noise and random time delay.

Figure 7. Performance of GA in handling model mismatch condition and random time delay.

VI. CONCLUSION

In this study, a benchmark of exothermic batch process model has been developed based on the work of Cott and Macchietto. Genetic algorithm is directly used as the controller to control the batch process temperature. It needs to calculate the suitable settings of heater power and coolant flow rate in order to maintain the reactor temperature at the desired trajectory. With the interest of testing the robustness of GA, variable time delay and disturbances are introduced into the simulation. The computational time of GA and some of the actuation delay are considered in simulation. The disturbance considered includes the measurement noises and model mismatch condition. From the simulation results, it can be concluded that the GA controller is able to provide an effective solution in controlling nonlinear exothermic process. In the future, performance of other methods can be investigated and compared with the performance of GA.

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