2012 Fourth International Conference on Computational Intelligence, Communication Systems and Networks

Genetic Algorithm based Multivariable Control for Exothermic Batch Process

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

***Abstract*—Exothermic process is highly nonlinear and complex process. Large amount of heat will be released during the chemical reaction. As a result of the exothermic behaviour, the reaction may become unstable and consequently poses safety concern to the plant if the reactor temperature exceeds the cooling capacity. In the industrial point of view, heating is needed in order to speed up the reaction rate so that it can reduce the overall process reaction time. Hence, this paper proposes genetic algorithm (GA) to control the reaction temperature as well as to balance the production needs with the safety specification. GA exploits probabilistic search method to optimise the specific objective function based on evolutionary principle. Simulation assessment of the GA has been carried out using a benchmark exothermic batch process model. The results show that GA is a good candidate in controlling the reactor temperature.**

Keywords-exothermic batch process; genetic algorithm; multivariable control

I. INTRODUCTION

Exothermic batch process has received foremost concentration over the recent years due to its flexibility to adapt to small volume production of various products (e.g. pharmaceuticals, polymers and etc) [1, 2]. Usually, reactor is heated up by using a heater in order to speed up the reaction rate, whereas it is cooled down by using coolant jacket in order to avoid thermal runaway [3, 4]. During the reaction, a large amount of heat is rapidly released when the reactants are being heated up. This continuous increase in temperature will cause the reaction becomes unstable and also will lead to thermal runway if the generated heat exceeds the cooling capacity of the reactor. As a result, the runaway reaction will pose significant safety risk to the plant personnel as well as the equipments [5]. The hazard associated with exothermic reaction is related to process specific factors, such as operating temperature, concentration and etc. Hence, developing a suitable control strategy to control the reactor temperature is the main task of this paper so that it can balance the production needs with the safety specification.

In industry, PID controller is still widely implemented due to its simplicity [6, 7]. Although the parameters of PID controller can be obtained by using some conventional tuning methods (e.g. Ziegler-Nichols method), it still needs an operator to manual re-tune the settings for aim to achieve the satisfactory responses. Regrettably, the optimum results are seldom obtained due to the need of operator's experiences. Hence, artificial intelligence techniques are introduced to reduce the dependency on human operator.

Genetic algorithm (GA) is a stochastic global search method that mimics the evolutionary process [8, 9]. 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 a very effective in finding optimal solutions for various nonlinear problems, such as in traffic control, robotics, power systems and etc. GA has been proposed to maximize the ergodic capacity for a given propagation scenario of MIMO antenna systems by obtaining the position and orientation of each MIMO array antenna [10]. The results show that some of the solutions found by GA were very subtle, which human operator would have difficulty to identify. Reference [11] has implemented GA to optimise traffic flow control system. In that paper, GA is taken the current traffic queue length as its input and then it will evolve out an optimised traffic light green time for the road intersection. In this work, GA is proposed to act directly as the controller to control 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 GA. The rest of the paper is organised as follows. Section II describes the mathematical modelling of batch process. Section III discusses the genetic algorithm. Section IV explains the simulation procedures. The performance of GA will be discussed in Section V. Finally, Section VI summarises the findings of this paper.

II. MODELLING OF BATCH REACTION

A benchmark batch process modelling proposed by Cott and Macchietto [12] is used in this research. It is assumed that a second-order, well-mixed, and irreversible liquid-phase exothermic reaction occurs in the process.

Reaction 1: $A + B \rightarrow C$
Reaction 2: $A + C \rightarrow D$

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

978-0-7695-4821-0/12 $26.00 © 2012 IEEE
DOI 10.1109/CICSyN.2012.17

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.

A. *Reference Temperature*

In the work of Cott and Macchietto [12], they found that the optimal isothermal reaction temperature is in the range of 90 °C to 100 °C. According to Kenneth *et al.* [13], 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 has to be perfectly regulated for a selected length of time. By considering the 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 it should be maintained at 95 °C until 120 minutes, as shown in Fig. 2.

B. *Mass Balance*

The law of conservation of mass is used to formula 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):

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

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 consumption/production rates for the substances are described in (2) and (3) respectively. In the findings of [14], 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.

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

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

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

Other physical parameters of reaction are shown in (4), (5) and (6).

$$W = \sum MW_i \cdot M_i, i = A, B, C, D \tag{4}$$

$$M_r = \sum M_i, i = A, B, C, D \tag{5}$$

$$C_{\rho r} = \frac{\sum \left(C_{\rho i} \cdot M_i\right)}{M_r}, i = A, B, C, D \tag{6}$$

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; $C_{\rho r}$ is average molar heat capacity; and $C_{\rho i}$ is molar heat capacity of substance i.

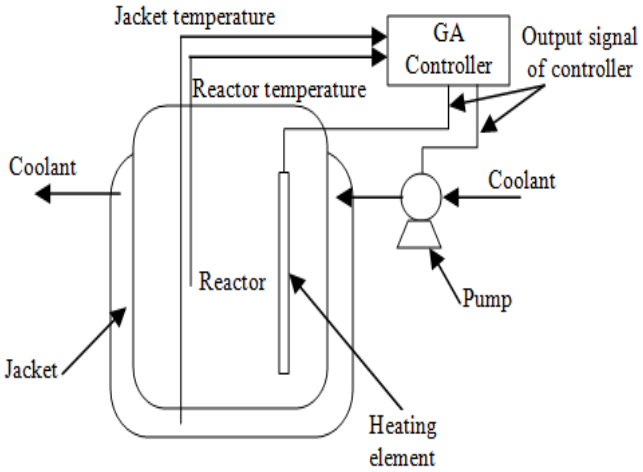


Figure 1. Batch process scheme.

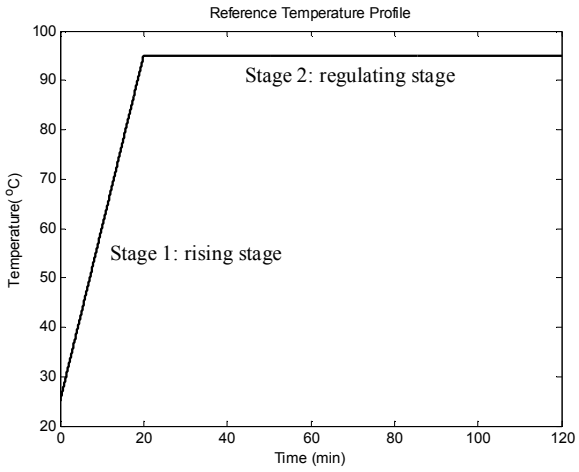


Figure 2. Reference temperature profile.

C. Thermal Energy Balance

The reactor temperature is influenced by the heater, exothermic heat released, and jacket temperature. Usually, the reactor temperature is higher than the jacket temperature, whereas the heater and the liberated heat will heat up the reactor. 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) and (8).

$$\begin{bmatrix} \dot{T}_r \\ \dot{T}_j \end{bmatrix} = \begin{bmatrix} \frac{1}{M_r C_{\rho r}} & 0 \\ 0 & \frac{(T_c - T_j)}{V_j} \end{bmatrix} \cdot \begin{bmatrix} Q_h \\ F_j \end{bmatrix} + \ldots \begin{bmatrix} \frac{1}{M_r C_{\rho r}} & \frac{-A_r(T_r - T_j)}{M_r C_{\rho r}} \\ 0 & \frac{A_r(T_r - T_j)}{V_j \rho_j C_{\rho j}} \end{bmatrix} \cdot \begin{bmatrix} Q_r \\ U \end{bmatrix} \quad (7)$$

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

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; $C_{\rho j}$ 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 for reaction i. All the model parameters are shown in Table I.

III. Genetic Algorithm

GA exploits probabilistic search method to optimise the specific objective function based on the evolutionary principle of survival of the fittest. GA has three basic operators, which are selection, crossover, and mutation. The framework of GA is shown in Fig. 3. The termination criterion is set as 10 generations.

A. Initialisation

In this paper, GA is used to search for the suitable heater power and coolant flow rate based on the reactor and jacket temperature. Initially, potential solutions are randomly generated. Each solution set is encoded in a string called chromosome. From the simulation data, the range of heater power is from 0 kW to 300 kW, whereas the range of coolant flow rate is from 0 liter/s to 1 liter/s. After a few times of testing, it is proved that the 50 population size of GA is enough for this study.

B. Fitness Evaluation

The fitness evaluation function interprets the chromosomes in term of physical representation and evaluates its fitness based on desired objective. This function is important since GA choose the optimal solution based on this evaluation fitness value. The fitness of each solution can be calculated by taking the reciprocal of the absolute error, since smaller error means that the solution is fitter. Hence the fitness function can represent as shown in (9).

$$J = 1 \Big/ \left| (T_{ref} - T_r) \right| \quad (9)$$

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 emphasise the fitter chromosomes by making duplicates of those chromosomes in hopes that their offspring will in turn have even higher fitness value, and eliminate those unfit chromosomes while maintaining the population size. Ranking selection method is used in this study because the best chromosomes do not differ much from others in term of being selected in matching pool.

First, all the chromosomes are sorted according to their fitness, from worst to best. The fittest chromosome will have higher ranking in this case. After that, implementation of this selection operator can be thought of as a roulette-wheel mechanism. The cumulative fitness of each chromosome is calculated by adding the individual ranked. Then, the selection probability is generated by multiply 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 to the matching pool. In this operation, the fittest chromosome will have larger range of cumulative fitness and hence it will have higher probability of being selected to the matching pool.

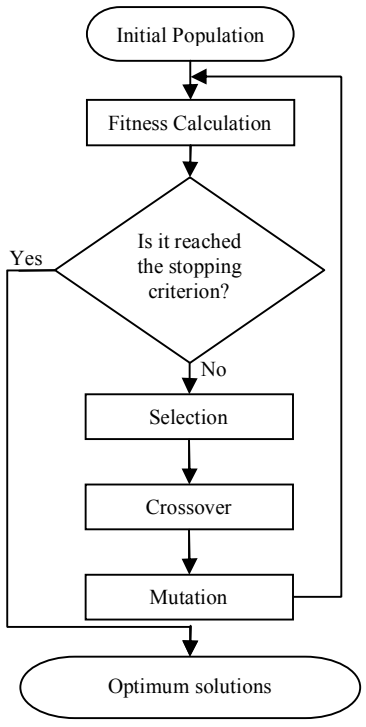


Figure 3. Framework of genetic algorithm.

D. Crossover

This operation is used to generate the new generation. In this operation, two chromosomes (called parents) are randomly picked up from matching pool. Then, some portions of the parents will exchange between each other and create two new chromosomes (called offspring). Blending method is used in this paper. This method combines 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).

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

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

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. That means only 90 % of chromosomes are used in the crossover operation and 10 % of the chromosomes are simply copied to the new generation.

E. Mutation

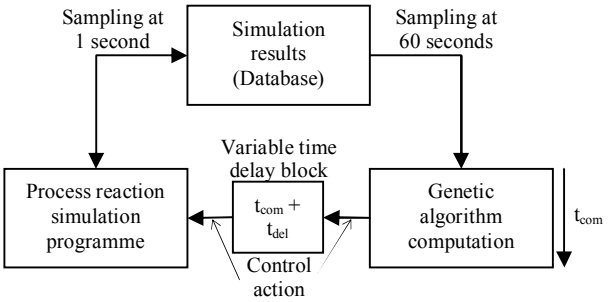
The mutation operator helps to prevent the searching trap in local maxima. However, the mutation probability should be kept low to prevent the loss of too many fit chromosomes and affect the convergence. Therefore, the mutation rate is set to 0.01 in this case. This paper is used random mutation, which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

IV. Simulation

All the modelling equations are simulated using MATLAB. The batch process simulation programme is run to obtain the relevant process measurement for every second, whereas the GA algorithm is sampled at the rate of 60 second. During the computation of GA algorithm, the process simulation programme is continuing run without waiting for GA solution. A stopwatch timer is used in MATLAB to measure the computational time delay of GA. The optimum solution calculated by GA is fetched into the simulation programme after computational time delay of GA. The actuation time delay is considered and introduced into simulation. The actuation time delay used in this paper is in the range of 20 seconds to 30 seconds. The flowchart of simulation is shown in Fig. 4.

Measurement errors are always present in 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 come out a first order moving average noise model equation to explain this condition, as shown in (12).

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



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

Figure 4. Simulation flowchart.

where a(k) is normally distributed at kth time interval; and Ti' is temperature after addition of measurement noise.

As stated in [15], 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 change is also equivalent to the presence of unmodelled reactions.

V. Results and Discussions

Fig. 5 shows the simulated performance of GA dealing with time delay and measurement noise in exothermic process. Fig. 6 shows the exothermic heat liberated during the reaction process. The control actions of GA for coolant flow rate and heating power are shown in Fig. 7 and Fig. 8 respectively.

In Fig. 5, it can be seen from the temperature responses profile that the GA able to bring the reactor temperature to the desired trajectory. At the beginning of the process, heating element is important to speed up the reaction rate in order to reduce the overall process cycle time. It can be shown in Fig. 7 that the heating power is around 200 kW during the first 20 minutes. At the same time, cooling system is needed because the exothermic heat is started release during the process. After 20 minutes, the exothermic heat

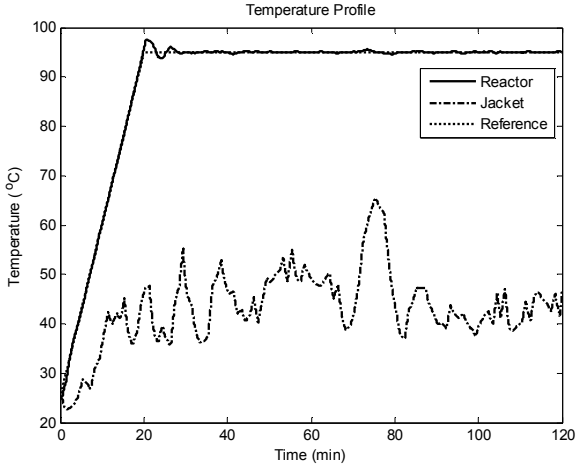


Figure 5. Performance of GA.

released is reduced. The heating and cooling system are only needed to maintain the temperature at 95 °C.

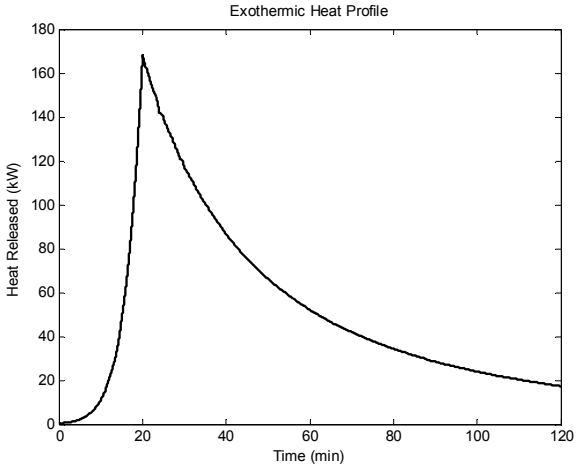


Figure 6. Exothermic heat released.

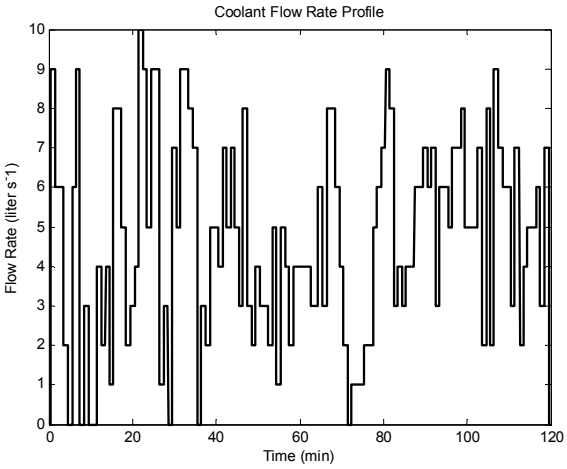


Figure 7. Optimal coolant flow rate profile.

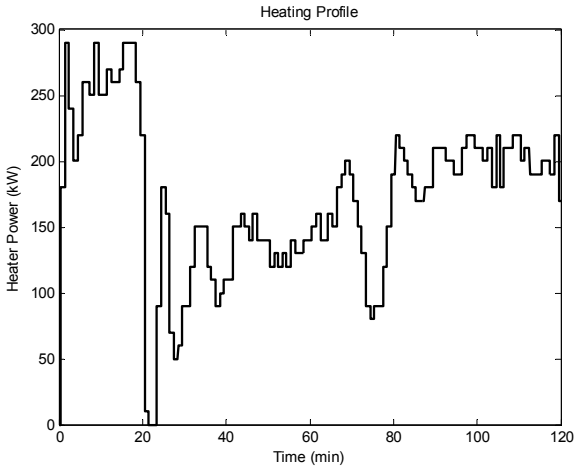


Figure 8. Optimal heating profile.

Fig. 9 shows the performance of GA under the model mismatch condition. Fig. 10 and Fig. 11 show the optimal profile of control action of GA under model mismatch.

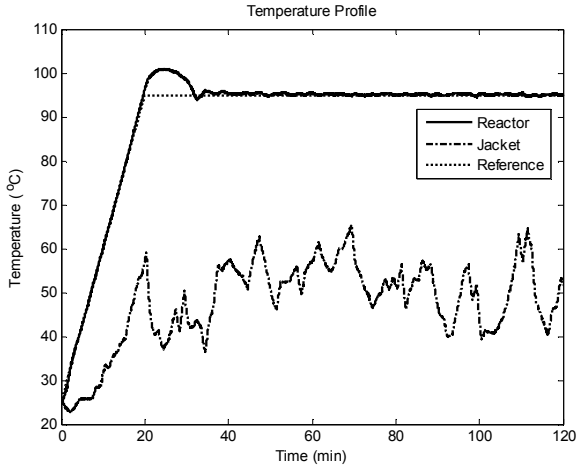


Figure 9. Performance of GA under model mismatch condition.

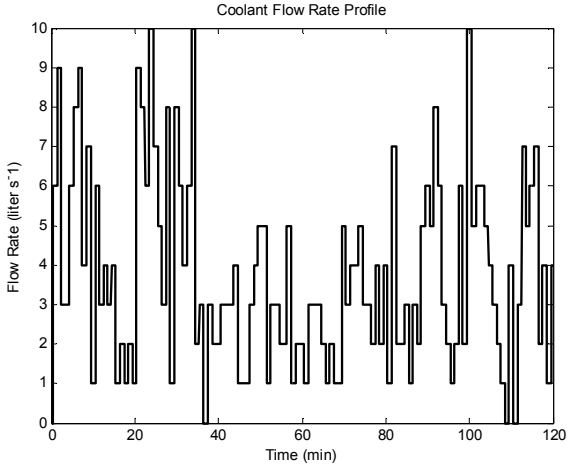


Figure 10. Optimal coolant flow rate under model mismatch condition.

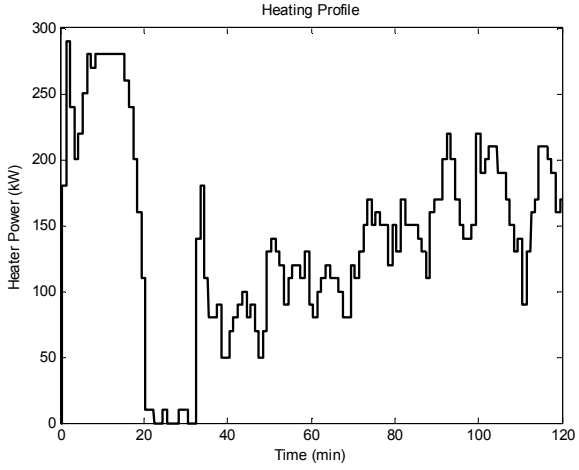


Figure 11. Optimal coolant flow rate profile under model mismatch condition.

Fig. 9 shows that the vigorous parameters change in the process will force the process towards instability. The GA reveals its robustness in control the process and able to prevent the runaway reaction. GA only gives a very small overshoot (5%) in the reactor temperature before the desired temperature is attained.

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. The GA needs to calculate the suitable settings of heater power and coolant flow rate in order to balance the production speed and safety specification. In the interest of express 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 time delay. And then the measurement noises and model mismatch condition. From the simulation results, it can be concluded that the GA controller able to provide an effective solution in controlling this nonlinear exothermic process. In the future, performance of other methods can be investigated and compared with the performance of GA.

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}	$kmol^{-1}$ s^{-1}	E_{a1}/k_B	10000	K
k_{02}	7.9×10^{16}	$kmol^{-1}$ 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			

ACKNOWLEDGMENT

The authors would like acknowledge the financial support of Universiti Malaysia Sabah (UMS) under Postgraduate Scholarship Scheme.

REFERENCES

[1] A.K.A. Wahab, M.A. Hussain, and R. Omar, "Development of PARS-EX Pilot Plant to Study Control Strategies," Control Engineering Practice, vol. 17, 2009, pp. 1220-1233, doi: 10.1016/j.conengprac.2009.05.008.

[2] K.M. Christensen, M.J. Pedersen, K.D. Johansen, T.L. Holm, T. Skovby, and S. Kiil, "Design and Operation of A Filter Reactor for Continuous Production of A Selected Pharmaceutical Intermediate," Chemical Engineering Science, vol. 71, 2012, pp. 111-117, doi: 10.1016/j.ces.2011.12.002.

[3] M.A. Hosen, M.A. Hussain, and F.S. Mjalli, "Control of Polystyrene Batch Reactors using Neural Network based Model Predictive Control (NNMPC): An Experimental Investigation," Control Engineering Practice, vol. 19, 2011, pp. 454-467, doi: 10.1016/j.conengprac.2011.01.007.

[4] M. Alipoor, M. Zeinali, and H.S. Yazdi, "Fuzzy Temperature Control in A Batch Polymerization Reactor using ANFIS Method," International Journal of Engineering and Technology, vol. 1, no. 1, 2009, pp.7-12.

[5] Hazard Investigation: Improving Reactive Harzard Management. US Chemical Safety and Hazard Investigation Board (CSB). 2002.

[6] M.K. Tan, Y.K. Chin, H.J. Tham, and K.T.K. Teo, "Genetic Algorithm based PID Optimization in Batch Process Control," Proc. 2011 IEEE International Conference on Computer Applications and Industrial Electronics (ICCAIE 2011), 2011, pp. 162-167, doi: 10.1109/ICCAIE.2011.6162124.

[7] Y. Wang, T. Liu, and Z. Zhao, "Advanced PI Control with Sample Learning Set-Point Design: Application on Batch Processes and Robust Stability Analysis," Chemical Engineering Science, vol. 71, 2012, pp. 153-165, doi: 10.1016/j.ces.2011.12.028.

[8] D. Mokeddem, and A. Khellaf, "Optimal Feeding Profile for A Fuzzy Logic Controller in A Bioreactors using Genetic Algorithm," Nonlinear Dynamics, vol. 67, no. 4, 2012, pp. 2835-2845, doi: 10.1007/s11071-011-0192-2.

[9] J.S. Yoon, Design of Real-Time Medium Access Control and The Optimization of End-to-End Delay using Genetic Algorithm, 2012. PhD Thesis. The City University of New York.

[10] M.O. Binelo, A.L.F. de Almeida, and F.R.P. Cavalcanti, "MIMO Array Capacity Optimization using a Genetic Algorithm," IEEE Transactions on Vehicular Technology, vol. 60, issue 6, 2011, pp. 2471-2481, doi: 10.1109/TVT.2011.2158460.

[11] K.T.K. Teo, W.Y. Kow, and Y.K. Chin, "Optimization of Traffic Flow Within an Urban Traffic Light Intersection with Genetic Algorithm," Proc. 2010 Second International Conference on Computational Intelligence, Modelling and Simulation (CIMSiM 2010), 2010, pp. 172-177, doi: 10.1109/CIMSiM.2010.95.

[12] B.J. Cott, and S. Macchietto, "Temperature Control of Exothermic Batch Reactors using Generic Model Control," Industrial and Engineering Chemistry Research, vol. 28, no. 8, 1989, pp. 1177-1184, doi: 10.1021/ie00092a010.

[13] T.T.K. Kenneth, S. Yaacob, R. Nagarajan, and G. Sainarayanan, "Certain Studies on Sample Time for A Predictive Fuzzy Logic Controller through Real Time Implementation of Phenol-Formaldehyde Manufacturing," Proc. 2004 IEEE Region 10 Conference (TENCON 2004), vol. 4, 2004, pp. 514-517, doi: 10.1109/TENCON.2004.1414983.

[14] R.A. Pulley, Batch Process Modelling Club Report CR 2828 (CON), 1986. Warren Spring Laboratory, Stevenage, Herts, UK.

[15] F. Caccavale, M. Iamarino, F. Pierri, and V. Tufano, Control and Monitoring of Chemical Batch Reactors. London: Springer-Verlag London Limited, 2011.