Genetic-Algorithm-Based Optimisation for Exothermic Batch Process

M. K. Tan, H. J. Tham and K. T. K. Teo

Abstract The aim of this chapter is to optimise the productivity of an exothermic batch process, by maximising the production of the desired product while minimising the undesired by-product. During the process, heat is liberated when the reactants are mixed together. The exothermic behaviour causes the reaction to become unstable and consequently poses safety issues. In the industries, a dual-mode controller is used to control the process temperature according to a predetermined optimal reference temperature profile. However, the predetermined optimal reference profile is not able to limit the production of the undesired by-product. Hence, this work proposed a genetic-algorithm-based controller to optimise the batch productivity without referring to any optimal reference profile. From the simulation results, the proposed algorithm is able to improve the production of the desired product and reduce the production of the undesired by-product by 15.3 and 34.4 %, respectively. As a conclusion, the genetic-algorithm-based optimisation performs better in raw materials utilisation as compared to the predetermined optimal temperature profile method.

Introduction

Batch process has been applied in the manufacturing industry due to its flexibility to handle various productions of high value-added product, such as specialty chemicals, agrochemicals, and pharmaceuticals. Although batch process is used

M. K. Tan (✉) · K. T. K. Teo
Modelling, Simulation and Computing Laboratory, School of Engineering and Information Technology, Universiti Malaysia Sabah, Jalan UMS 88400 Kota Kinabalu, Sabah, Malaysia
e-mail: msclab@ums.edu.my

H. J. Tham
Chemical Engineering Programme, School of Engineering and Information Technology, Universiti Malaysia Sabah, Jalan UMS 88400 Kota Kinabalu, Sabah, Malaysia
e-mail: hjtham@ums.edu.my

R. Pogaku et al. (eds.), *Developments in Sustainable Chemical and Bioprocess Technology*, DOI: 10.1007/978-1-4614-6208-8_27,

for various types of production, quite often the common aim is to optimise the production of the desired product while at the same time minimising the waste. Since there is no inflow and outflow during the process, the raw materials utility is fully relied on the reactor temperature especially for the exothermic reaction (Nisenfeld 1996). In exothermic reactions, heat is liberated during the process hence consequently increases the reactor temperature. If the liberated heat is higher than the plant cooling capacity, the reaction will become unstable and, hence, poses a safety issue to the plant personnel (Hazard Investigation 2002).

Previously, batch productivity optimisation for exothermic process was obtained by controlling the reactor temperature according to a predetermined optimal temperature profile (Mujtaba et al. 2006; Sujatha and Pappa 2012; Tan et al. 2011). Although they can control the reactor temperature to follow the desired trajectory effectively, the aim of minimising the waste may not be achieved. Besides, the global price competition and escalating raw materials costs have also urged the batch industries to consider an effective way of utilising the raw materials (Fernandez et al. 2012).

For these reasons, genetic algorithm (GA) is introduced to optimise the exothermic batch productivity. This work reports the performance of a GA in exothermic batch process optimisation without referring to any reference values. The performance of the proposed GA is then compared with the conventional dual-mode controller (DM) which uses the predetermined optimal temperature profile.

Methodology

Batch Process Modelling

A benchmark batch process model, developed by Cott and Macchietto (1989), is used in this study. It is assumed that a two-parallel, well-mixed, and irreversible liquid-phase exothermic reactions occur in the process, as shown in below.

$$\text{Reaction 1} : \text{A} + \text{B} \rightarrow \text{C} \qquad \text{Reaction 2} : \text{A} + \text{C} \rightarrow \text{D}$$

where A and B are the raw materials, C is the desired product, and D is the undesired by-product. Initially, all the raw materials are charged into the reactor and left to react for 120 min. The jacket surrounding the reactor is used to control the reactor temperature. Figure 1 illustrates the schematic of the batch process system.

The dynamic modelling of a batch process can be divided into two parts: component balance and energy balance. The law of conservation of mass is applied to model the component balance of the reactor contents. The production/consumption rate of all substances and each component balance are described in (1) and (2), respectively.

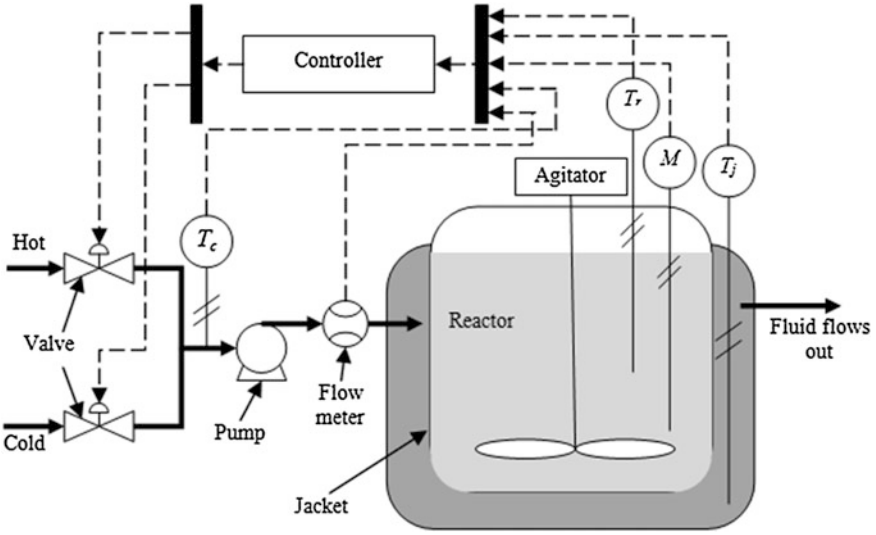

Fig. 1 Schematic of batch process system

$$\begin{bmatrix} R_1 \\ R_2 \end{bmatrix} = \begin{bmatrix} k_1 & M_A & M_B \\ k_2 & M_A & M_C \end{bmatrix} \tag{1}$$

$$\begin{bmatrix} \dot{M}_A \\ \dot{M}_B \\ \dot{M}_C \\ \dot{M}_D \end{bmatrix} = \begin{bmatrix} -1 & -1 \\ -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} R_1 \\ R_2 \end{bmatrix} \tag{2}$$

where R_i is the reaction rate of Reaction i, k_i is the reaction rate constant of Reaction i, M_j is the molar concentration of substance n, and $\dot{M}_n$is the changing rate of substance n.

Since both the reactions are temperature dependence, the reaction rate constant for both reactions can be modelled using Arrhenius equation, as shown in (3).

$$k_i = k_{oi} \exp\left(\frac{-E_{ai}}{R \cdot T_r}\right), \text{ where } i = 1, 2 \tag{3}$$

where k_{oi} is the frequency factor of Reaction i, E_{ai} is the activation energy of Reaction i, R is the gas constant, T_r is the reactor temperature in unit Kelvin.

On the other hand, the energy balance of the reactor and jacket are shown in Eqs. (4) and (5), respectively.

$$\frac{\mathrm{d}T_r}{\mathrm{d}t} = \frac{\left(Q_{\text{exo}} + Q_j\right)}{M_r C_{\rho r}} \tag{4}$$

$$\frac{dT_j}{dt} = \frac{F_j \rho_j C_{\rho j}\left(T_c - T_j\right) - Q_j}{V_j \rho_j C_{\rho j}} \tag{5}$$

where Q_{exo} and Q_j are the exothermic heat released and heat transferred from jacket to reactor, respectively, M_r is total molar concentration of reactor contents, $C_{\rho r}$ is the heat capacity of reactor contents, T_j and T_c are the jacket and fluid temperature, respectively, F_j is the fluid flow rate, ρ_j is the fluid density, $C_{\rho j}$ is the heat capacity of the fluid, and V_j is the volume of the jacket.

Q_{exo} and Q_j can be defined as shown in (6) and (7), respectively. Here, the initial temperature for T_r and T_j are assumed to be 25 °C.

$$Q_{exo} = \Sigma(-\Delta H_i R_i), \text{where } i = 1, 2 \tag{6}$$

$$Q_j = UA_r\left(T_j - T_r\right) \tag{7}$$

where ΔH_i is the enthalpy change of Reaction s, U is the heat transfer coefficient between the jacket and reactor, A_r is the surface area of reactor conducts with the jacket.

Other important physical variables of the process are described in (8) and (9), respectively, where n = A, B, C, D. The plant parameters can be taken from Tan et al. (2011).

$$M_r = \Sigma M_n \tag{8}$$

$$C_{pr} = \frac{\Sigma\left(C_{\rho n} \cdot M_n\right)}{M_r} \tag{9}$$

where $C_{\rho n}$ is the heat capacity of substance n.

Genetic Algorithm Modelling

The GA proposed for the optimisation is based on the biological evolution theory and Darwin's natural selection concept: "survival of the fittest". In this case, it is used to manipulate the jacket inlet fluid temperature, $T_{c,}$ with a sampling time of 60 s. First, the real number chromosome representation technique is applied to represent the potential solutions (fluid temperature). After a few trials, results showed that a population size of 50 is enough in this work. The manipulated variables are bounded in the range of 0–120 °C.

Each chromosome is then evaluated by a fitness function in order to distinguish their suitability to the process optimisation. In this work, the fitter chromosome is able to maximise the production of the desired product while minimise the undesired product. The optimisation function, J, as defined in (10) is applied to evaluate the fitness of each chromosome. The chromosome with high fitness value will receive preferential treatment in procreation process later. Ranking selection

technique is implemented to select the chromosomes into a mating pool so that the mating pool will not be dominated by those high fitness value chromosomes.

$$\max_{T_c} J = \int \Delta M_c dt - 6.25 \int \Delta M_D dt \tag{10}$$

During the crossover operation, two chromosomes (parents) are randomly selected from the mating pool. Then, with a probability of 90 %, both selected parents will exchange some of their information with each other and create two new chromosomes (offspring), whereby they have 10 % chance to duplicate into new generation. The blending (arithmetic) technique is employed in this crossover operation, as expressed in (11) and (12). The first offspring generated using this technique is merely the compliment of the second offspring.

$$x_1 = \beta \cdot P_1 + (1 - \beta) \cdot P_2 \tag{11}$$

$$x_2 = (1 - \beta) \cdot P_1 + \beta \cdot P_2 \tag{12}$$

where x_i is the offspring i, P_i is the parent i, and β is the random number in [0, 1].

The newly created offspring will have a 1 % chance to be mutated in order to avoid the potential solutions being trapped in the local maxima. During the mutation, a new chromosome is randomly selected from the entire solution space. The evolutionary process is stopped when 10th generation is reached, and it will return the optimal fluid temperature to the plant.

Results and Discussions

In this study, the consumption rate of the limiting reactant (substance A) is limited to 7.855 kmol so that the optimisation performance of the proposed GA and the DM can be compared equitably. The configuration of the DM is taken from Cott and Machietto (1989), which is well tuned for this case. The optimisation performance of GA and DM are shown in Fig. 2a and b, respectively.

In general, one cycle of batch process can be divided into three stages. At the beginning of the process (first stage), the reactor contents should be heated up to a certain temperature to enable the chemical reactions to take place. This happens during 0–10 min when full heating is given to the reactor and before the production starts. It can be observed from Fig. 2a-ii that the fluid temperature determined by GA is not a smooth straight line during this period compared to the DM, as shown in Fig. 2b-ii. This is because GA is a stochastic search method that searches the optimal solution through the entire solution space. In some cases, such as a batch process, there is not only one optimal solution in the solution space, and hence, it affects the GA output response to have a small fluctuation.

The second stage can be categorised as the stage where the reaction rate increases rapidly. This is the critical stage due to the huge amount of exothermic heat being released and causes the reactor temperature to increase rapidly. Hence,

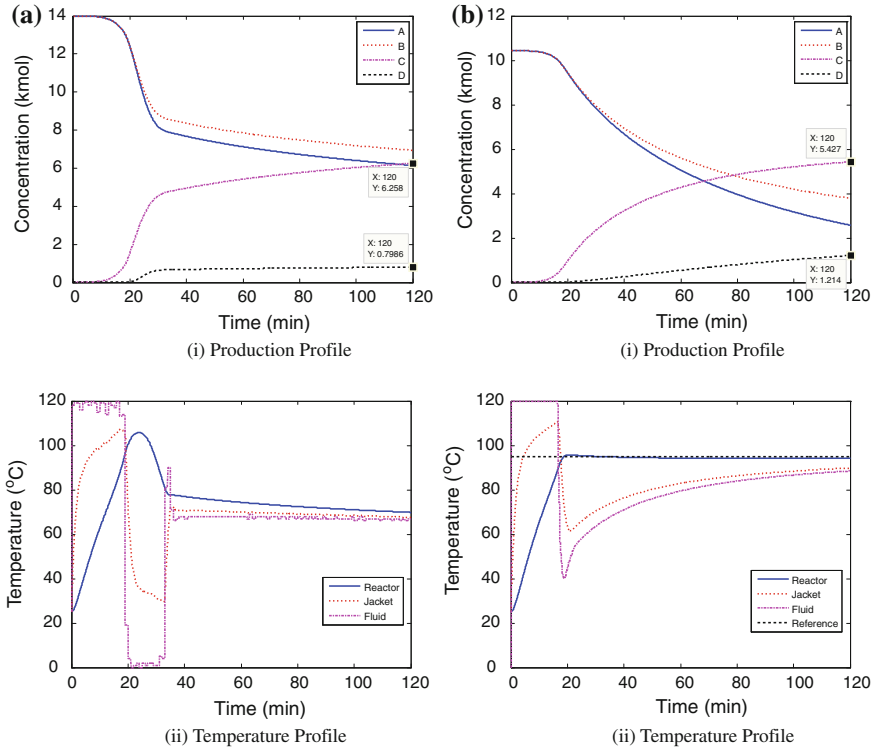

Fig. 2 Performance of genetic algorithm and dual-mode controller

the cooling system plays an important role in order to avoid the thermal runaway. The results show that the reaction starts when the reactor temperature is around 60 °C, as shown in Fig. 2a-ii and b-ii at 10 min. During the first part in this stage, both controllers continue to give full heating to the reactor whereas the cooling is given during the second part of this stage. For GA, the full heating is given during 10–20 min in order to speed up the production rate using high temperature, as shown in Fig. 2a, whereas the DM only gives full heating during 10–18 min with the purpose of increasing the reactor temperature up to the reference point in the shortest time, as shown in Fig. 2b. It can also be observed from the results that the waste production started at 20 min, when the temperature is high. In order to limit the waste production, GA proposes full cooling during 20–30 min. Conversely, DM tried to maintain the reactor temperature at the desired trajectory, rather than limit the waste production. Therefore, the waste is produced linearly from 20 min until the batch ends, as shown in Fig. 2b-i.

In the last stage, the GA seems to be slowly reducing the reactor temperature in order to limit the waste production, and at the same time, ensuring the production of desired product is increased, as shown in Fig. 2a.

Table 1 Performance of the proposed genetic algorithm and the conventional dual-mode controller in optimising the batch productivity

	Genetic algorithm	Dual-mode controller
Product C (kmol)	6.258	5.427
Undesired product D (kmol)	0.799	1.214

The overall performance show that the GA is able to harvest 6.258 kmol of desired product C and 0.796 kmol of undesired by-product D, whereas the DM only harvests 5.427 kmol of desired product C and 1.214 kmol of undesired by-product D. The results show that the desired product harvested by the GA is 15.3 % more than the DM, whereas the waste produced by the GA is 34.4 % less than the DM. Table 1 summaries the performance of the proposed GA and the conventional DM controller to optimise the batch productivity.

Conclusions

In this chapter, GA is proposed to optimise the raw materials utility for an exothermic batch process without referring to any optimal temperature profile. The performance of the developed GA is examined using a benchmark exothermic batch process model. The results show that the proposed method can perform better than the conventional DM which follows an optimal temperature profile. In future, the work will be focusing on optimising the GA development in handling various uncertainties and to improve the robustness of GA.

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

References

Cott, B. J., & Macchietto, S. (1989). Temperature control of exothermic batch reactors using generic model control. *Industrial and Engineering Chemistry Research, 28*(8), 1177–1184.

Fernandez, I., Renedo, C. J., Perez, S. F., Ortiz, A., & Manana, M. (2012). A review: Energy recovery in batch processes. *Renewable and Sustainable Energy Reviews, 16*(4), 2260–2277.

Hazard Investigation. (2002). Hazard Investigation: Improving reactive hazard management. U.S. Chemical Safety and Hazard Investigation Board. Washington, U.S.

Mujtaba, I. M., Aziz, N. & Hussain, M. A. (2006). Neural network based modelling and control in batch reactor. *Chemical Engineering Research and Design 84*(A8), 635–644.

Nisenfeld, E. (1996). *Batch control: Practical guides for measurement and control*. North Carolina: American Technical Publishers.

Sujatha, S., & Pappa, N. (2012). Performance of gain scheduled generic model controller based on BF-PSO for a batch reactor. *Asian Journal of Scientific Research, 5*(2), 31–44.

Tan, M. K., Tham, H. J. & Teo, K. T. K. (2011). PID-based temperature control for exothermic chemical reactor using hybrid QL-GA. In: 18th Regional Symposium on Chemical Engineering, 27–28 Oct, Ho Chi Minh City, Vietnam.