Exothermic Batch Process Optimisation via Multivariable Genetic Algorithm

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***Abstract*—This paper aims optimise the exothermic batch productivity while minimise the waste production by manipulating the fluid temperature and fluid flow rate. During the process, a large amount of heat is 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. Commonly, the optimisation of the batch process is based on the predetermined optimal reference temperature profile. However, this reference profile is unable to limit the waste production effectively. Therefore, multivariable genetic algorithm (MGA) is proposed in this work to optimise the productivity of the process without referring to the predetermined reference profile. The results show that the MGA is able to harvest more than 80 % of yield in handling human error and equipment failure.**

Keywords-batch process; optimisation; genetic algorithm; multivariable

I. INTRODUCTION

Batch process has attracted attentions compared to continuous process due to its flexibility to handle various productions of high value-added product in small-volume, such as specialty chemicals, agrochemicals, pharmaceuticals and etc. Although the batch process is able to adapt with various production types, there is only one common aim which is to optimise the production of desired product while minimising the waste. Since there is no inflow and outflow during the batch process, the raw materials utility of batch process is fully relied on the reactor temperature especially for the exothermic reaction [1]. The high reactor temperature will cause the reaction becomes faster and consequently release more exothermic heat. The heat released will further increase the reactor temperature, and may cause the reaction becomes unstable and hence will lead to thermal runaway if it is not well controlled. As a result, the runaway reaction will pose safety concern to the plant personnel.

Nowadays, the global price competition and escalating raw materials costs have urged the batch industries to consider an effective way of utilising the raw materials [2]. Besides, the product quality is regularly impaired by the occurrence of undesired by-product [3]. Various optimisation methods have been proposed in literature to maximise the yield of the batch process.

In the past, a pre-determined optimal reactor temperature profile is used for the process control to maximise the productivity [4]. However, it is difficult to measure the process variables and to determine the optimal set-point in practical due to the nature characteristics of the batch process. These will tend to cause the optimal trajectory to swift with the time changing.

To cope with the time-varying process, various intelligent algorithms have been considered in chemical processes for the optimisation problem. Knowledge-based fuzzy logic control has been implemented to settle the process ambiguity problem [5]. Optimisation through this control requires thorough understanding of the process to set the rules and membership functions to obtain desired process output. Alternatively, neural network can work in pair with fuzzy control to map the process variables relationship via sufficient data training [6]. Another way, genetic algorithm can work in pair with the fuzzy logic to auto-tune the fuzzy logic membership function range [7]. Besides that, other intelligent control systems, such as predictive control [9] and Q-learning [9], are developed using the black-box model concept to tackle the process optimisation problem.

In this work, multivariable genetic algorithm (MGA) is proposed to maximise the production of desired product while minimise the production of waste. MGA was attempted to determine the optimal jacket inlet fluid temperature and the optimal fluid flow rate profile under the several case studies. Here is interested in reporting the robustness of MGA in handling optimisation problem without referring to any reference profile. The hazards associated with exothermic reaction are related to the process specific factors, such as improper charging, human error, equipment failure and parameter variant, are considered in the robustness studies.

II. MODELLING OF BATCH PROCES

The batch process model used in this paper is based on the work of Cott and Machietto [10]. It is assumed that two parallel, well-mixed, and irreversible liquid-phase exothermic reactions occur in the process. The stoichiometric equations of the reactions are shown in the (1) and (2).

$$\text{Reaction 1: } A + B \rightarrow C, \quad \Delta H_1 = -41840 \text{ kJ kmol}^{-1} \qquad (1)$$

$$\text{Reaction 2: } A + C \rightarrow D, \quad \Delta H_2 = -25105 \text{ kJ kmol}^{-1} \qquad (2)$$

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where A and B are the raw materials, C is the desired product, D is the undesired by-product, and ΔH_i is the enthalpy change of Reaction *i*.

The plant consists of a reactor with a jacket, as shown in Fig. 1. Initially, the raw materials (12 kmol each) are loaded into the reactor and the reaction starts when the agitator begins to stir the substances. On the other hand, the jacket with fluid flowing in it is used to control the reactor temperature.

The proposed algorithm is implemented as the controller to optimise the batch productivity by manipulating the jacket inlet fluid temperature and the fluid flow rate. The main control objective in this work is to maximise the percentage of yield at the end of the batch. Fig. 2 illustrates the block diagram of batch process optimisation via the MGA. The modelling of batch process is explained as follows:

A. Reaction Rate Modelling

The reaction rate modelling equations are derived from the law of mass action, which basically can be divided into two terms. The first term is the temperature-dependent term which can be described by Arrhenius equation, whereas the second term is the composition-dependent term which is proportional to the product of the molar concentration of the reactants. Generally, the reaction rate for the Equation 1 and Equation 2 can be described in (3) and (4) respectively.

$$R_1 = k_1 \cdot e^{\left(\frac{-E_1}{(k_B \cdot T_r)}\right)} \cdot M_A^{\ 1} \cdot M_B^{\ 1} \tag{3}$$

$$R_2 = k_2 \cdot e^{\left(\frac{-E_2}{(k_B \cdot T_r)}\right)} \cdot M_A^{\ 1} \cdot M_C^{\ 1} \tag{4}$$

where E_i is the activation energy of Reaction *i*, k_B is the Boltzmann constant, k_i is the frequency factor of Reaction *i*, M_n is the molarity of substance *n*, R_i is the reaction rate of Reaction *i*, and T_r is the reactor temperature in unit Kelvin.

B. Component Balance Modelling

The component balance modelling equations are derived from the law of conservation of mass. Since the reaction utilises the reactants to create product, the component changing rate of reactant will be indicated in a negative-sign, conversely the component changing rate of product is indicated in a positive-sign. Hence, the instantaneous molarity changes of the reactor contents are expressed in (5).

$$\begin{bmatrix} \dot{M}_A \\ \dot{M}_B \\ \dot{M}_C \\ \dot{M}_D \end{bmatrix} = \begin{bmatrix} -1 & -1 \\ -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} R_1 \\ R_2 \end{bmatrix} \tag{5}$$

where $\dot{M}_n$ is the molarity changes of substance *n*.

C. Energy Balance Modelling

In general, the reactor and the jacket can be treated as two separate closed systems. The energy balance modelling for these two closed systems can be derived from the first law of thermodynamics. The (6) and (7) describes the energy balance in the reactor and jacket respectively, where the (8) explains the exothermic heat released during the reaction.

$$M_r C_{\rho r} \frac{dT_r}{dt} = Q_{exo} + UA_r(T_j - T_r) \tag{6}$$

$$V_j \rho_j C_{\rho j} \frac{dT_j}{dt} = UA_r(T_r - T_j) + F_j \rho_j C \rho_j (T_c - T_j) \tag{7}$$

$$Q_{exo} = \sum_{i=1}^{2} \left(-\Delta H_i \cdot R_i\right) \tag{8}$$

where A_r is the surface area of reactor that contacts with jacket, C_{pj} and $C_{\rho r}$ is the heat capacity of the fluid and reactor contents respectively, F_j is the jacket inlet fluid flow rate, Mr is total molarity of reactor contents, is the heat capacity of reactor contents, ρ_j is the fluid density, Q_{exo} is exothermic heat released, T_c, T_j, and T_r and are the fluid, jacket and reactor temperature respectively in unit degree Celsius, U is the heat transfer coefficient between reactor and jacket.

$\alpha + \beta = \chi.$ (1) (1)

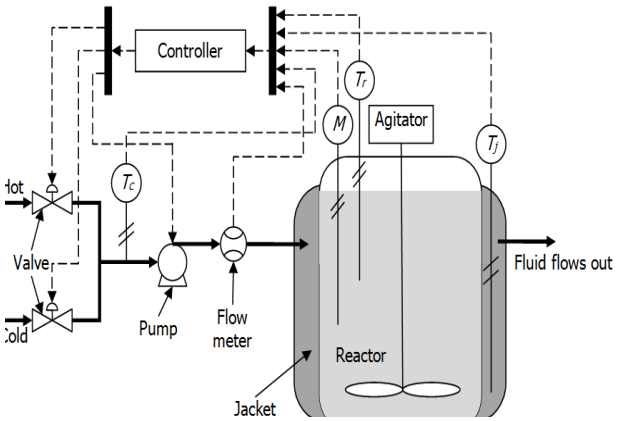


Figure 1. Schematic diagram of batch process.

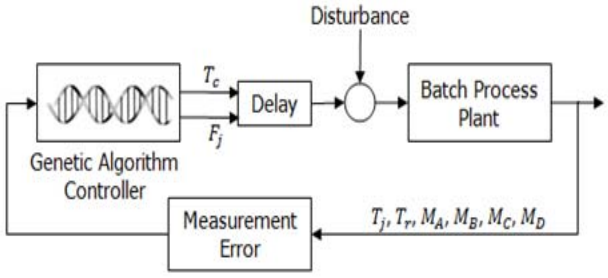


Figure 2. Block diagram of batch process optimisation via multivariable genetic algorithm.

D. Physical Parameters Modelling

The total reactor contents molarity and heat capacity of the reactor contents are described in (9), and (10) respectively. The process parameters can be obtained from [11].

$$M_r = \sum (M_n) \tag{9}$$

$$C_{\rho r} = \frac{\sum (C_{\rho n} \cdot M_n)}{M_r} \tag{10}$$

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

III. Development of Multivariable Genetic Algorithm

MGA is proposed to optimise the batch productivity based on the biological evolution theory and Darwin's natural selection concept: "survival of the fittess". The proposed algorithm will search the optimal fluid temperature, T_r, and flow rate, F_j, profile heuristically for the process. It is assumed that the fluid temperature is bounded in the range of 10 °C to 120 °C, whereas the fluid flow rate is bounded in the range of 0 m^3 s^{-1} to 0.01 m^3 s^{-1}. The framework of MGA is shown in Fig. 3. The anatomy of the developed MGA is discussed as follows:

A. Chromosome Representation

In this work, real-number chromosome representation technique is applied to encode the potential solutions (combination of fluid temperature and flow rate) into a string called chromosome because this technique requires minimum space storage and faster computing time compared to binary chromosome representation. The chromosome structure of the developed MGA is shown in Fig. 4. After few times of testing, it shows that 50 population size is enough for this work.

B. Fitness Function

The fitness function evaluates the fitness of each chromosome based on the optimisation strategy, as expressed in Equation (11). From the equation, it shows that the fitter chromosome should have higher production in desired product and lower production in the undesired waste.

$$\max_{T_c \,\&\, F_j} J(t) = \beta_1 \int_{t-1}^{t+1} \dot{M}_c dt - \beta_2 \int_{t-1}^{t+1} \dot{M}_D dt \tag{11}$$

where β_1 and β_2 are the weight factors.

C. Selection

The selection mimics the nature selection concept, which is survival of the fittest. In this stage, the fitter chromosomes will receive preferential attention to form a mating pool for the later reproduction process. This stage emphasises the fitter chromosomes are remained in the mating pool at the expense of those unfit chromosomes.

Here, rank selection is used in order to avoid the mating pool is dominated by fittest chromosome. This is because of if the mating pool is dominated by a certain chromosome, then it will affect the exploration of GA to search for the suitable solution.

D. Reproduction

The reproduction consists of crossover and mutation operator, as shown in Fig. 3. In this work, the blending technique is used in crossover operator. Two parents are randomly selected from the mating pool and create two new offspring using the (12) and (13). The probability of crossover is set as 0.9. This predefined probability allows the both selected parents to have 90 % chances to exchange their information with each other, and 10 % chances to remain unmodified in the next generation. The main target of the selection is to hope that the newly offspring will in turn better than the parents.

$$offspring\_1 = [\alpha \times parent\_1] + [(1-\alpha) \times parent\_2] \tag{12}$$

$$offspring\_2 = [(1-\alpha) \times parent\_1] + [(\alpha) \times parent\_2] \tag{13}$$

On the other hand, the mutation operator is responsible to keep diversity in the population. It helps to avoid the potential solutions to trap in local optimum. However, the probability of mutation must be kept low to prevent the loss of too many fit chromosome and consequently affect the convergence of the solutions. Hence, this work uses 1 % mutation rate.

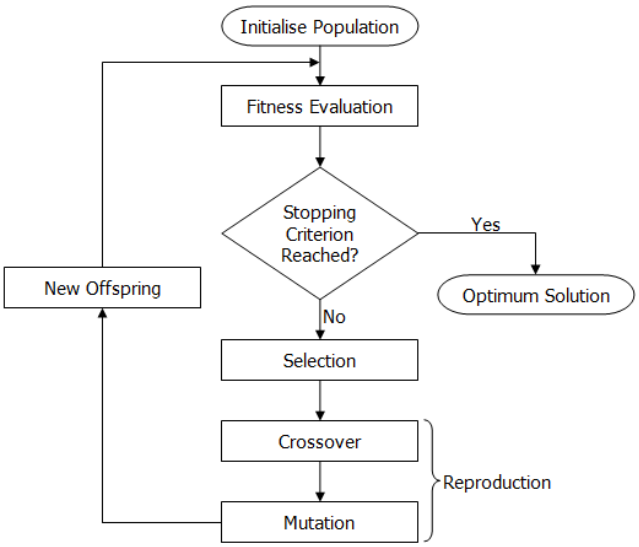


Figure 3. Framework of mulivaraiable genetic algorithm.

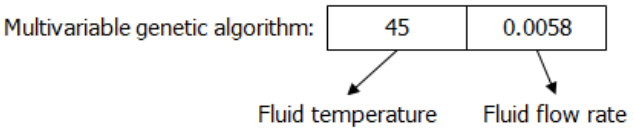


Figure 4. Structure of chromosome.

E. Termination Criteria

The evolution will keep on going, where the new generation replace the old generation and breed the third generation, until the preset stopping criterion is achieved. Here, the termination criterion is set as 10 generations, after that the evolutionary process will stop and return the optimal fluid temperature and flow rate to the process plant. The performance of the MGA is evaluated by the (14).

$$yield = \frac{\text{total amount of desired product}}{\text{total amount of limiting reactant consumed}} \times 100\ \% \quad (14)$$

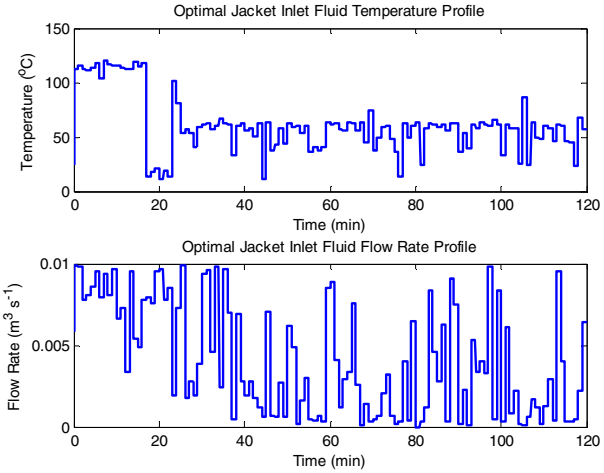
IV. Results and Discussions

The model of the exothermic batch process is modelled and simulation in MATLAB m-file. The process simulation programme is run at the rate of 1 sec, whereas the MGA programme is sampled at the rate of 60 sec. The proposed algorithm is tested under four cases, named as nominal case, improper charging, temporary insufficient cooling and parameter variant.

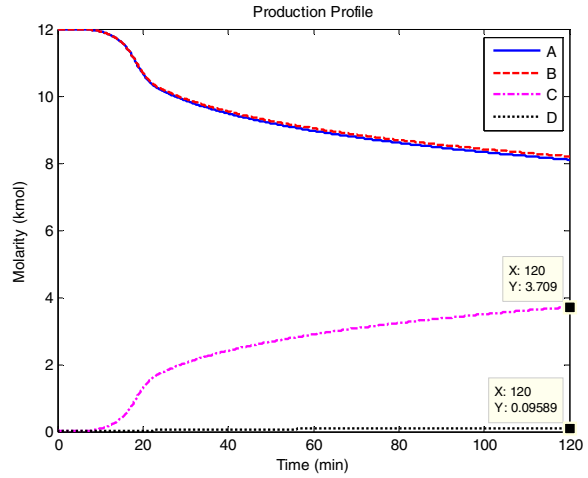
The improper charging simulates the factor which involves the abnormalities of the raw material concentration. This factor is caused by the human error [12]. In this case, it is assumed that the initial concentration of the raw materials is 16 kmol. The temporary insufficient cooling simulates the partially blockage in the inlet fluid piping which is caused by the equipment failure [12]. In this case, it is assumed that the fluid flow rate becomes 0.001 $m^3\ s^{-1}$ during 18 min to 22 min. The last case simulates the parameter variant condition. This work assumes that the frequency factors and the activation energy in (3) and (4) are ± 3 % from the nominal value. Other than the above mentioned, random time delay and temperature measurement errors are introduced in all the cases, except the nominal case. In this work, the random time delay is assumed in the range of 5 sec to 15 sec, whereas the measured temperature will have a precision of ± 0.5 °C.

The performance of the MGA in nominal case is shown in Fig. 5. At the beginning of the process, the MGA gives a preheating to the reactor in order to accelerate the reaction. During 18 min to 21 min, the MGA gives a full cooling to compensate the exothermic heat released during the process. After 20 min, the MGA tries to maintain the reactor temperature at around 65 °C in order to limit the waste production. The fluctuation in the output responses of MGA, as shown in Fig. 5(a), is caused by the inherent heuristic search characteristic of MGA because sometimes there is not only one optimal solution can be found in solution space.

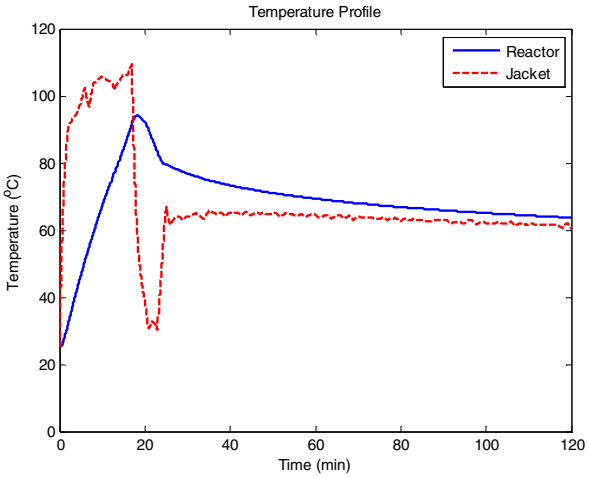
The performance of the proposed MGA in handling the improper charged condition is shown in Fig. 6. According to the Law of Mass Action, increase in the reactant concentration will increase the reaction rate and hence increase the exothermic heat released as well. Since the exothermic heat released is larger than the nominal case, the full cooling period given in this case should be longer than



(a) Control actions of multivariable genetic alogrithm



(b) Production profile



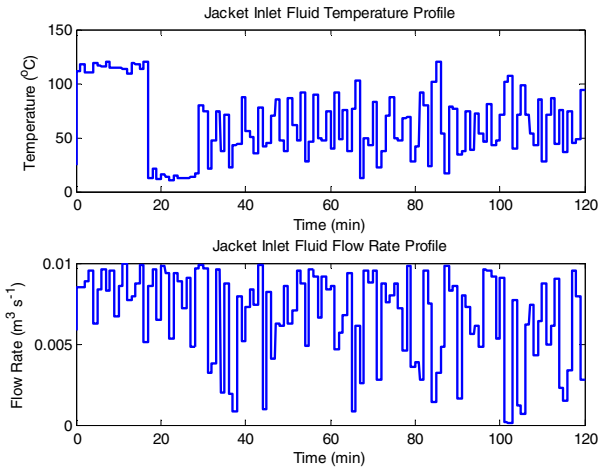
(b) Temperature profile

Figure 5. Performance of multivariable genetic algorithm in nominal case.

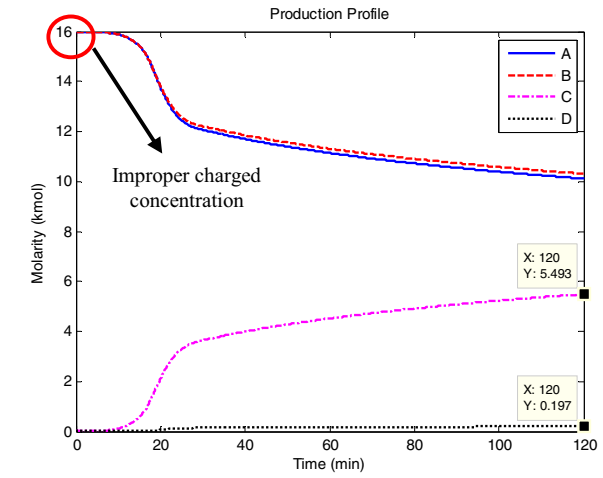
the nominal case. Therefore, it can be noticed from the Fig. 6(a) that the MGA gives a full cooling from 18 min to 30 min, which is 8 min longer compared to the nominal case, in order to compensate the high amount of heat released during the reaction. The Fig. 6(b) shows that the total amount of desired product C obtained at the end of the batch is 5.493 kmol, or equivalent to 48.1 % higher than the nominal case. This is because of the high amount of initial charged will increase the probability of the successful reaction hence more product is produced. Again, in order to limit the waste production, the MGA will maintain the fluid temperature at around 60 °C.

Fig. 7 shows the performance of proposed MGA in handling the sudden insufficient cooling condition during 18 min to 21 min. This period is a critical period to have the cooling system because the exothermic heat is released rapidly during this period, as discussed in previous. Therefore, this test is to examine the robustness of MGA to control the process once the fault is over. Since the jacket inlet fluid is partially blocked, it will limit the flow rate of the fluid hence lead to the insufficient cooling circumstance. As a result, the heat released will increase the reactor temperature and cause the more waste to produce. After the fault is over, the MGA took 9 min (until 30 min) to limit the waste production by bringing down the reactor temperature. At the end of the batch, as shown in Fig. 7(b), the total waste produced is 0.4519 kmol, or equivalent 371.27 % higher than the nominal case.

Although the proposed MGA is performed well in handling the human fault and equipment failure circumstances, it does not be capable to deal with the parameter variant condition, as shown in Fig. 8. The Fig. 8(b) shows that the MGA is unable to limit the waste production efficiently because the proposed MGA is using the predetermined and non-adaptable model in the fitness function to determine the suitability of the potential solutions. The Table I summarises the productivity of the proposed MGA in all the case studies.

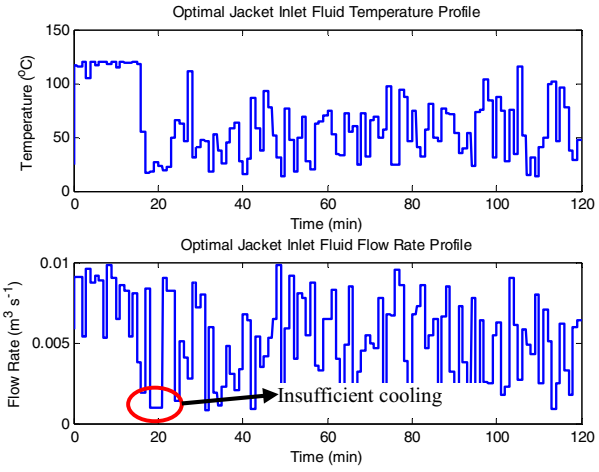


(a) Control actions of multivariable genetic alogrithm

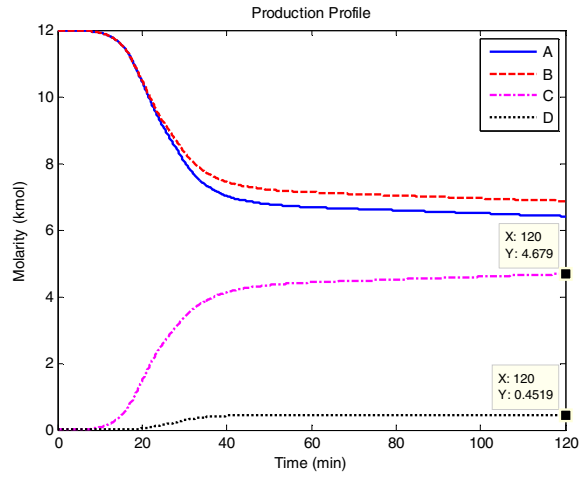


(b) Production profile

Figure 6. Performance of multivariable genetic algorithm in charging failure condition.

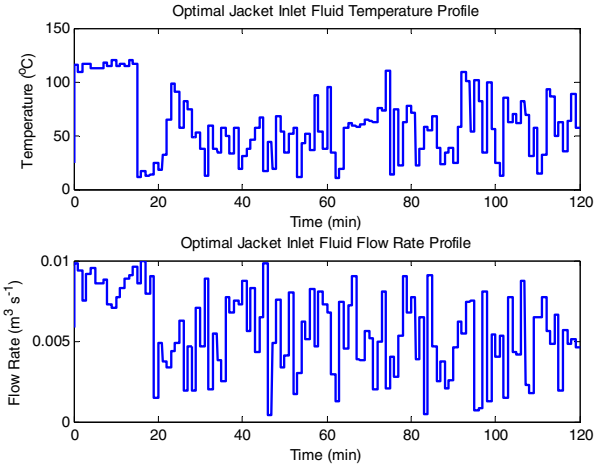


(a) Control actions of multivariable genetic alogrithm

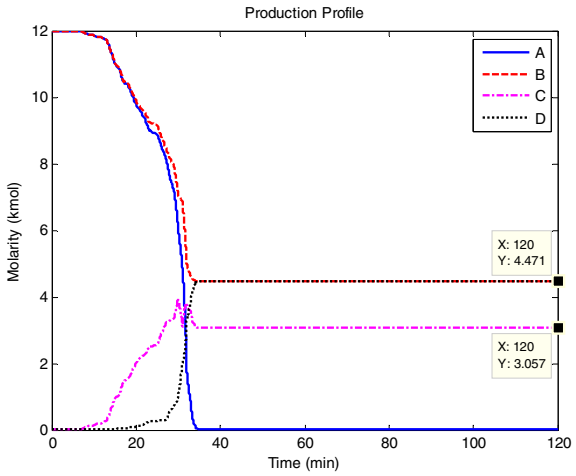


(b) Production profile

Figure 7. Performance of multivariable genetic algorithm in temparory pump failure condition



(a) Control actions of multivariable genetic alogrithm



(b) Production profile

Figure 8. Performance of multivariable genetic algorithm in parameter variant condition.

TABLE I. PROCESS MODELLING PARAMETERS

Case	Product C (kmol)	Undesired Product D (kmol)	Yield (%)
Nominal	3.709	0.09589	95.08
Improper charging	5.493	0.197	93.31
Pump failure	4.679	0.4519	83.81
Parameter variant	4.471	3.057	25.48

V. CONCLUSION

In this study, a benchmark of exothermic batch process model has been as the case study. Multivariable genetic algorithm (MGA) is proposed to optimise the productivity of an exothermic batch process by manipulating fluid temperature and fluid flow rate. The optimisation aim of the developed algorithm is to maximise the production of the desired product while minimise the production of the undesired by-product. The simulation results show that the proposed MGA is able to optimise the process with the yield more than 80 % in handling human error and equipment failure condition. However, the proposed method is unable to cope with the parameter variant circumstance due to the predetermined and non-adaptable model in fitness function is used to determine the suitability of the potential solutions. In future, this research will be focusing on improve the MGA by adding the adaptive feature into its fitness function in order to improve its flexibility to cope with parameter variant condition.

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