Evolutionary Optimization Scheme for Exothermic Process Control System

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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 minimizing the production of undesired by-product. During the process, a large amount of heat is released rapidly when the reactants are mixed together due to exothermic behavior. This 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. This paper proposes genetic algorithm (GA) as an approach to control the process temperature by changing the coolant temperature because GA does not require the exact process dynamics in advance, which normally in practical, the process dynamics are poorly known in practical. GA is able to evolve itself to obtain an optimum solution to change the coolant temperature. The simulation studies show that the GA will be a good candidate to optimize the process and minimize the temperature overshoot throughout the reaction process. Furthermore, GA is able to evolve itself to obtain an optimum solution to change the coolant temperature.**

Keywords – dynamic optimization; exothermic process; temperature control; genetic algorithm

I. INTRODUCTION

Batch process reveals several characteristics that make it become an interesting topic in process control systems. It 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.), and also its suitability to carry out with dangerous reactions. In general, batch process is aim to maximize the yield of desired product while minimize the production of undesired by-product in a finite duration of process. Usually, the purity and quality of the desired product cannot be measured directly during the process. As a result of that, procses supervision is commonly based on direct measureable quantities, such as temperature [1]. In order to maximize the desired yield and minimize the process time, the reactor temperature is adjusted based on the pre-determined optimal temperature profile.

Exothermic batch temperature control is proved to be a challenging control task because a large amount of heat is released rapidly when the reactants are mixed together during the process. This will cause unstable reaction and it will consequently affect the purity and quality of the desired product [2]. In the previous studies, many techniques are proposed to control the reactor temperature, such as dual-mode (DM) technique, generic model control (GMC) technique, adaptive technique, predictive technique and etc [3, 4, 5, 6]. It can be concluded that most of the studies were using model based controllers, which is highly dependent on a precise plant model. However, in practical, the detailed dynamic model of most reaction systems is poorly known. Therefore, model based controllers will normally experience difficulties in process control if there are an unpredictable changes in operating condition and model mismatch occurred throughout the process.

The purpose of this paper is to present a reliable non-model based controller technique to improve the batch operation performance while avoiding model mismatch situations. To stress the effectiveness of the proposed control technique, genetic algorithm (GA) is tested using a developed batch reactor model to adapt the PID parameters to replace human operating PID.

The organization of this paper is described as follows. Section II describes the plant modelling. Section III explains the proposed optimization scheme. Section IV shows the performance of the proposed control technique. Finally, Section V summarizes the findings in this paper.

II. PLANT MODELLING

The dynamic modelling of the batch process used in this research is based on the model and parameters proposed by [7]. A parallel, well-mixed liquid phase reaction is considered here, 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 react together and produce desired product C, whereas the Reaction 2 is the side reaction where reactant A

reacts with product C produce undesired by-product D. Fig. 1 illustrates the batch reactor diagram.

A. Thermal Energy Balance

Exothermic heat released during the process will further increase the reactor temperature. In order to maintain the reactor temperature in a desired trajectory, it should be cooled down using the jacket surrounding the reactor, as shown in Fig. 1. The change of reactor temperature can be described as (3).

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

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 hotter place to heat up the colder place.

$$\frac{dT_j}{dt} = \frac{F_j \rho_j C_{\rho_j}(T_{in} - T_j) - UA(T_j - T_r)}{V_j \rho_j C_{\rho_j}} \tag{4}$$

Initially, the reactor, jacket and coolant temperature are assumed to be same 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 [7].

B. Mass Balance

The reaction rate constants for Reaction 1 and Reaction 2 are highly dependent on the reactor temperature through the Arrhenius equation, as shown in (5) and (6) respectively.

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

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

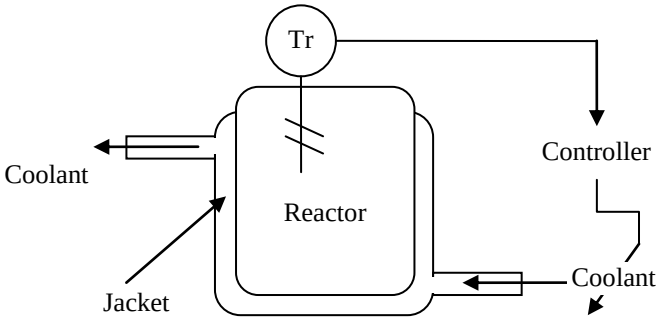


Figure 1. Batch reactor diagram

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

$$R_1 = k_1 M_A M_B \tag{7}$$

$$R_2 = k_2 M_A M_C \tag{8}$$

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 respectively, 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.

$$\frac{dM_A}{dt} = -R_1 - R_2 \tag{9}$$

$$\frac{dM_B}{dt} = -R_1 \tag{10}$$

$$\frac{dM_C}{dt} = R_1 - R_2 \tag{11}$$

$$\frac{dM_D}{dt} = R_2 \tag{12}$$

C. Physical Parameters

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

$$M_r = M_A + M_B + M_C + M_D \tag{13}$$

$$C_{\rho_r} = C_{\rho_A} M_A + C_{\rho_B} M_B + C_{\rho_C} M_C + C_{\rho_D} M_D \tag{14}$$

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.

The proposed technique consists of two components: optimization scheme and controller. In the optimization scheme, genetic algorithm (GA) is proposed as the controller parameters optimizer because GA does not need to have prior knowledge about the plant. It wills evolve towards the best controller parameters by observing the reactor temperature changes [8].

On the other hand, PID controller is proposed as the controller in this paper because it is still commonly used 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 from GA optimizer.

A. Optimization Scheme

The framework of the GA is shown in Fig. 2. First, an initial population of solutions is randomly generated with a population size of 50. Since the output of this GA function are optimum PID parameters, the solutions of GA are strings of just three parameters, which is able to completely characterize all PID parameters, as shown in Fig. 3.

Then, the fitness of each solution is calculated by using the estimated plant parameters. The best solution obtains highest fitness value; otherwise, it will obtain lower fitness value. The equation of fitness function is described in (15).

$$Fitness = \frac{1}{(T_{ref} - T_{est})^2} \tag{15}$$

where T_{ref} and T_{est} are the reference temperature and the estimated process temperature respectively.

In the selection operation, ranking method is used. This operation emphasizes 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 keeping the population size as constant.

In crossover operation, blending method is used with a rate of 0.9. This operation will randomly pick two solutions, called parent solutions, from the mating pool. Some portions of the parent solutions will be exchanged and create two new solutions, which is called offspring. This method combines variable values form the two parents into new variable values in the offspring. The first offspring variable value comes from a combination of two corresponding parent variable values. The second offspring is merely the complement of the first offspring. Equation (16) and (17) are used to create the offspring solutions.

$$x_{n1} = \beta \cdot x_{p1} + (1-\beta) \cdot x_{p2} \tag{16}$$

$$x_{n2} = \beta \cdot x_{p2} + (1-\beta) \cdot x_{p1} \tag{17}$$

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

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

The stopping criterion of GA is whenever the maximum number of generation is reached. The maximum number of generation is set to 10. Hence, the GA will stop after 10 generations and returns the optimal PID parameters to PID controller.

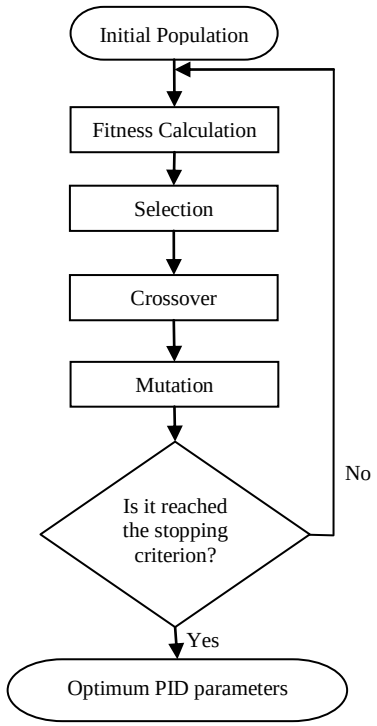


Figure 2. Framework of Genetic Algorithm

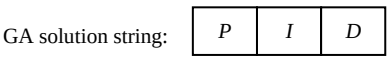


Figure 3. GA Solution String

B. Controller

The controller model is based on PID control algorithm, as described in (18).

$$u(t) = K_p e(t) + K_i \int_0^t e(\tau) d\tau + K_d \frac{de(t)}{dt} \tag{18}$$

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

IV. RESULTS AND DISCUSSION

The performance of the optimization scheme for adaptive PID controller has been compared with the traditional fixed PID controller. First of all, PID parameters are manually tuned using all the nominal plant parameters and Fig. 4 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 situation. The reactor temperature is rose to the desired temperature set point in 20 min times with less than 0.1 square errors. The released exothermic heat during the process is shown in Fig. 5.

However, it is very important to test the robustness of the controller with incoming fault because the reactor must always be operated in safe condition in regard of any faults. Therefore, the traditional PID controller with the well tuned parameters in nominal case is tested under two aspects: change in process parameters and model mismatch. The robustness of PID is then compared with the robustness of the proposed technique.

The first test involves 16.7 % reductions in the initial nominal reactants concentration (MA and MB). This test represents changes in operating condition caused by an accidental failure in charging system. The second test involves a reduction in 25.0 % reduction in the nominal heat transfer coefficient and 25.0 % increase in nominal reaction rate of Reaction 1, which are due to fouling in the heat transfer surface and model mismatch respectively.

In practice, inherent variable time delay is one of the main challenges for the process controller to react efficiently [9]. Therefore, random time delay is introduced at the controller output due to the valve delay occurred in the jacket inlet stream and controller calculation time [10].

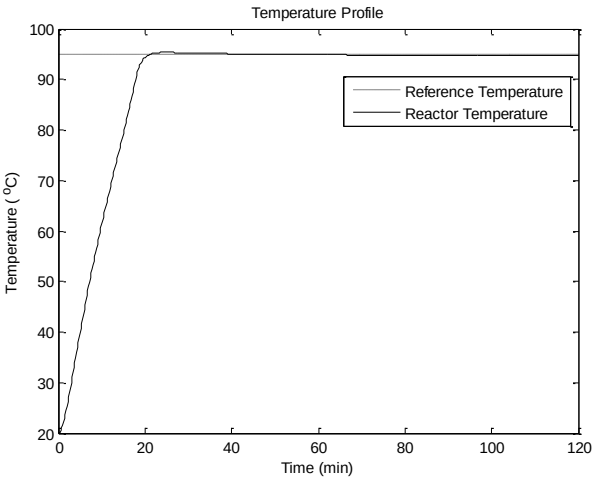


Figure 4. Performance of PID controller at nominal case

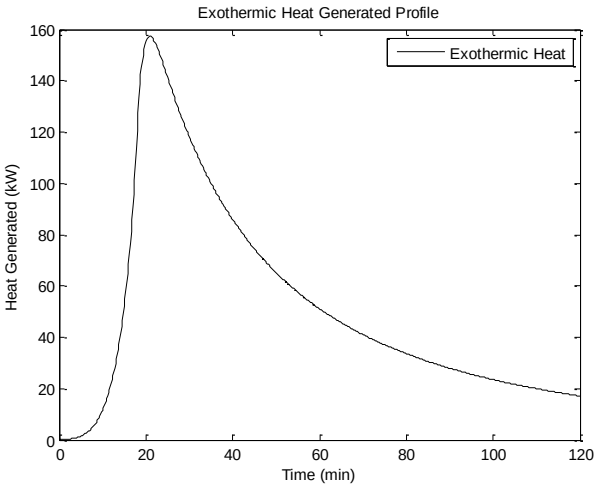
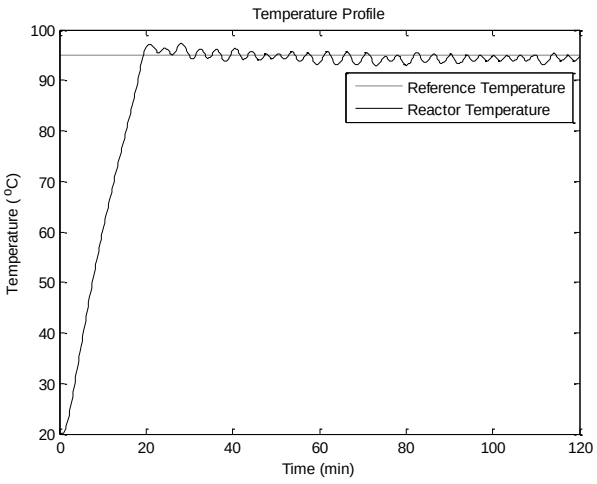


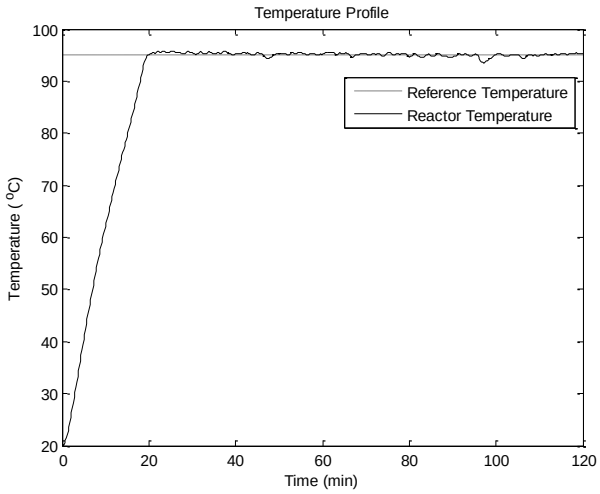
Figure 5. Exothermic heat profile under nominal case

Fig. 6a and Fig. 6b shows the performance of PID and the proposed GAPID under the change in operating condition, first robustness test respectively. The simulation result shown in Fig. 6 illustrates that the performance of PID always oscillates around the reference temperature, whereas the GAPID technique is able to adapt the PID parameters and control the reactor temperature according to the reference temperature.

Fig. 7a and Fig. 7b show the performance of PID and GAPID under the mismatch model situation, second robustness test respectively. The simulation results show that the traditional PID controller is not suitable to control the process if the model parameters are suddenly varied from the nominal condition. The overshoot temperature is up to 180 °C or equivalent to 50.0 % higher than the sustainable range of the system, which is only 120 °C. However, GAPID is capable to maintain the reactor temperature in the sustainable range of the system and cool down the reactor to the desired trajectory in a shorter period. From the results, it can be concluded that the proposed technique is able to control the temperature more robustly as compared to the traditional PID controller in in overcoming the internal disturbances.

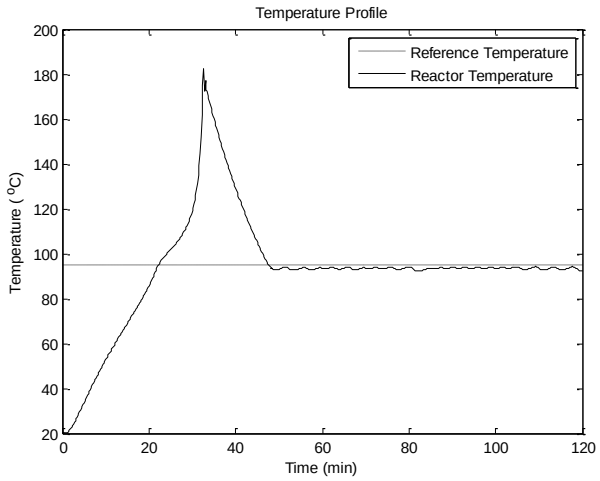


(a)

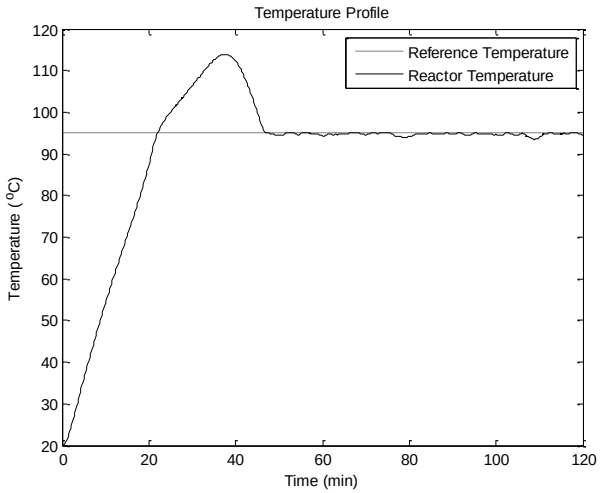


(b)

Figure 6. Performance of controllers for change in operating condition: (a) performance of PID, (b) performance of GAPID



(a)

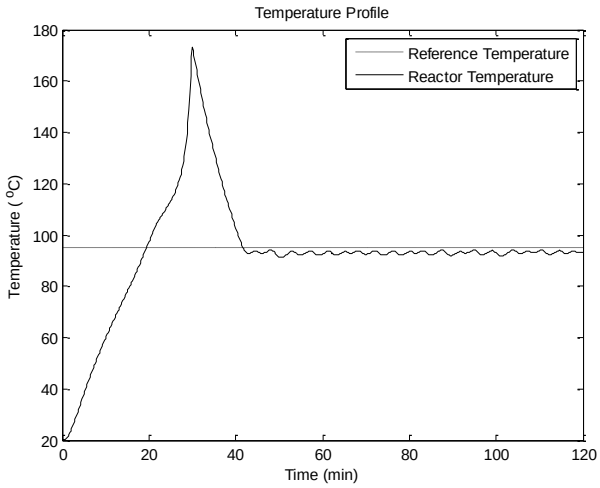


(b)

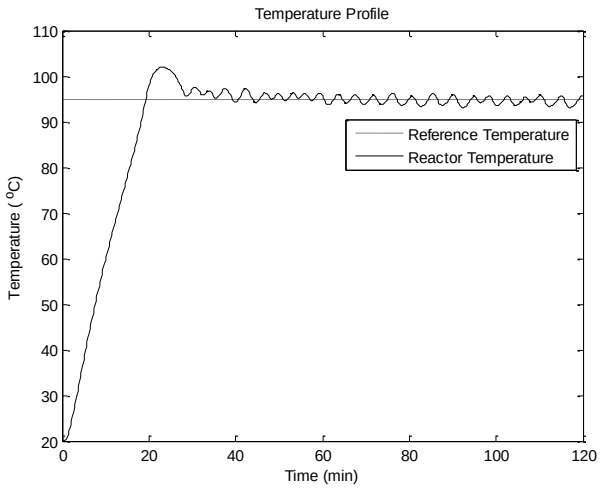
Figure 7. Performance of controllers for model mismatch: (a) performance of PID, (b) performance of proposed control technique

Fig. 8 highlights the robustness of the traditional PID controller and GAPID in overcoming the external disturbance and variable time delay. The external disturbance involves a reduction in coolant flow rate to 0.001 m^3 s^{-1} during the time 18 min to 21 min where this is a critical period since a large amount of exothermic heat is released during this period, as shown in Fig. 5. This situation represents a sudden block in the valve and hence limits the flow rate of coolant.

As a results, Fig. 8 shows the simulation results show that the traditional PID has poor performance in control the temperature when the external disturbance is introduced, whereas the proposed control technique is able to maintain the reactor temperature within the sustainable range of the system and then able to control the temperature to the desired trajectory after the valve recovers to normal condition.



(a)



(b)

Figure 8. Performance of controllers for external disturbance: (a) performance of PID, (b) performance of proposed control technique

V. CONCLUSION

In this study, an exothermic plant model with evolutionary optimization scheme of PID controller has been developed based on the characteristic of batch process. The proposed control technique consists of two components: optimization scheme and controller. GA is used in the optimization scheme to optimize and adapt PID parameters, whereas traditional fixed PID controller is used to control the reactor temperature by manipulating the coolant temperature. From the simulation performances, it can be verified that the proposed optimization scheme provides an acceptable temperature control due to its robustness against the variable time delay, change in nominal operating condition and model mismatch situations. In future, GA can be used to optimize the flow rate of coolant and the reactor temperature in order to maximize the yield of desired product while minimizing the production of undesired by-product.

APPENDIX

TABLE I. MODELLING PARAMETERS AND DESCRIPTION

Parameter	Value	Unit	Description
A	Refer to (4)	m^2	Conduction surface between jacket and reactor
$C_{\rho A}$	75.31	kJ $kmol^{-1}$ $°C^{-1}$	Molar heat capacity of substance A
$C_{\rho B}$	167.36	kJ $kmol^{-1}$ $°C^{-1}$	Molar heat capacity of substance B
$C_{\rho C}$	217.57	kJ $kmol^{-1}$ $°C^{-1}$	Molar heat capacity of substance C
$C_{\rho D}$	334.73	kJ $kmol^{-1}$ $°C^{-1}$	Molar heat capacity of substance D
$C_{\rho j}$	1.8828	kJ kg^{-1} $°C^{-1}$	Heat capacity of coolant
$C_{\rho r}$	Refer to (3)	kJ $kmol^{-1}$ $°C^{-1}$	Total molar heat capacity
Fj	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_{in}	-	°C	Coolant temperature
T_j	-	°C	Jacket temperature
T_r	-	°C	Reactor temperature
U	0.6807	kW m^{-2} $°C^{-1}$	Heat transfer coefficient
V_j	0.6912	m^3	Volume of jacket

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