GENETIC ALGORITHM FOR CONTROL AND OPTIMISATION OF EXOTHERMIC BATCH PROCESS

TAN MIN KENG

SCHOOL OF ENGINEERING AND INFORMATION TECHNOLOGY
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TAN MIN KENG

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Tan Min Keng
PK2010-8093

CERTIFICATION

NAME : **TAN MIN KENG**

MATRIC NO. : **PK2010-8093**

TITLE : **GENETIC ALGORITHM FOR CONTROL AND OPTIMISATION OF EXOTHERMIC BATCH PROCESS**

DEGREE : **MASTER OF ENGINEERING (ELECTRICAL AND ELECTRONIC ENGINEERING)**

VIVA DATE : **1st FEBRUARY 2013**

DECLARED BY

Signature

1. **SUPERVISOR**
   Mr. Kenneth Teo Tze Kin

2. **CO-SUPERVISOR**
   Dr. Tham Heng Jin

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ABSTRACT

GENETIC ALGORITHM FOR CONTROL AND OPTIMISATION OF EXOTHERMIC BATCH PROCESS

The aim of this research is to control and optimise the production of the desired product while minimising the waste production for an exothermic batch process. 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, dual-mode controller (DMC) is employed in the industries to control the process. However, this approach is not robust in dealing with sudden disturbance. Hence, various advanced control strategies have been introduced. In general, most of the studies use predictive approach to estimate the process behaviour and a slave controller, usually proportional-integral-derivative (PID), is employed to control the process based on the estimated plant behaviour. Nevertheless, these methods require huge batch of data for tuning its parameters. Therefore, genetic algorithm (GA) is proposed in this work since precise mathematical model is not required. Although the proposed genetic algorithm controller (GAC) is able to regulate the process temperature to the desired path, it does not limit the waste production effectively. As such, another approach, GA is proposed to optimise the productivity without referring to a predetermined profile, namely genetic algorithm optimiser (GAO). The results show that GAO is able to improve the yield ratio from 0.77 to 0.97 or approximate 25.0 % as compared to the GAC. Further evaluations have shown that GA with predetermined fitness function is unable to cope with the environmental changes. As a result, improved multivariable genetic algorithm (IMGA) with adaptable fitness function ability is introduced in this work. Results show that the IMGA is able to improve the yield ratio from 0.25 to 0.79 as compared to GAO in handling the parameter variant conditions.

ABSTRAK

Tujuan kajian ini adalah untuk mengawal dan mengoptimumkan pengeluaran produk yang dikehendaki sambil meminimumkan pengeluaran bahan buangan untuk proses kelompok yang bersifat eksotermik. Semasa proses tersebut, tenaga haba yang sangat tinggi akan dibebaskan apabila bahan tindak balas dicampurkan bersama. Sifat eksotermik ini akan menjejaskan kestabilan tindak balas dan seterusnya membahayakan keselamatan pekerja. Biasanya, pengawal dua mod (DMC) digunakan dalam industri untuk mengawal proses tersebut. Namun, pendekatan ini tidak mantap dalam pengendalian gangguan yang mendadak. Oleh itu, pelbagai strategi kawalan maju telah diperkenalkan. Secara umum, kebanyakan kajian menggunakan pendekatan ramalan untuk menganggarkan perilaku proses dan seterusnya pengawal-hamba, biasanya pengawal PID, digunakan untuk mengawal proses berdasarkan anggaran tersebut. Walau bagaimanapun, kaedah ini memerlukan pangkalan data yang besar untuk menyelaraskan parameternya. Oleh itu, algoritma genetik (GA) dicadangkan dalam kerja ini kerana ia tidak memerlukan model matematik yang tepat. Sungguhpun pengawal algoritma genetik (GAC) yang dicadangkan berupaya untuk mengawal suhu proses mengikut laluan yang dikehendaki, ia tidak dapat mengurangkan pengeluaran sisa dengan berkesan. Justeru itu, pendekatan lain, iaitu pengoptimum algoritma genetic (GAO) dicadangkan untuk mengoptimumkan produktiviti tanpa merujuk kepada profil yang telah ditetapkan. Keputusan menunjukkan bahawa GAO mampu meningkatkan nisbah hasil dari 0.77 ke 0.97 atau lebih kurang 25.0 % berbanding dengan GAC. Penilaian lanjut menunjukkan bahawa GA dengan fungsi kecergasan pratentu tidak dapat menangani perubahan sekeliling. Dengan itu, algorithma genetik berbilang pembolehubah bertambah baik (IMGA) diperkenalkan dalam kerja ini. Keputusan menunjukkan bahawa IMGA dapat meningkatkan nisbah hasil dari 0.25 ke 0.79 berbanding dengan GAO dalam menangani keadaan variasi parameter.

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LIST OF ABBREVIATIONS

AI	Artificial intelligence
ANN	Artificial neural network
ANFIS	Adaptive-neuro fuzzy inference system
CSB	United States Chemical Safety Board
DMC	Dual mode controller
EKF	Extended Kalman filter
FL	Fuzzy logic
GA	Genetic algorithm
GAC	Genetic algorithm controller
GMC	Generic model controller
HSE	Health and Safety Executive of United Kingdom
IMGA	Improved multivariable genetic algorithm
ISE	Integral squared error
LV-MPC	Latent variable model predictive control
MGAC	Multivariable genetic algorithm controller
MGAO	Multivariable genetic algorithm optimiser
MPC	Model predictive control
NMPC	Nonlinear model predictive control
NNMPC	Neural network based model predictive control
PID	Proportional-integral-derivative controller
PSO	Particle swarm optimisation
SAPF	Self-adaptive predictive function
SVM	Support vector machine

LIST OF SYMBOLS

α	Random number in arithmetic crossover
β_1	Weight factor 1 of optimisation function
β_2	Weight factor 2 of optimisation function
ρ	Reactor contents density
ρ_j	Fluid density
ΔH_i	Reaction heat of Reaction i
ΔM_i	Molar concentration changing rate of substance i
Δt	Change in time
a_{est}	Estimated process parameter
A_r	Surface area of reactor conducts with the jacket
b_{est}	Estimated process parameter
c_{est}	Estimated process parameter
C_{ρ_i}	Heat capacity of substance i
C_{ρ_j}	Heat capacity of fluid
C_{ρ_r}	Heat capacity of reactor contents
D	Derivative-parameter of PID
d_{est}	Estimated process parameter
E_i	Activation energy of Reaction i
E_m	Temperature error setting of dual-mode controller
F_j	Fluid flow rate
h	Height of reactor
I	Integral-parameter of PID
J	Optimisation function

k	Reaction rate constant
k_B	Boltzmann constant
k_i	Reaction rate constant of Reaction i
k_{0_i}	Frequency factor of Reaction i
K_1	GMC tuning constant 1
K_2	GMC tuning constant 2
KE	Kinetic energy
m	Counter
M_i	Molar concentration of substance i
$\dot{M}_i$	Molar concentration changing rate of substance i
M_r	Total molar concentration of reactor contents
MW_i	Molecular weight of substance i
N	Number of chromosome
P	Proportional-gain of PID
PE	Potential energy
PL	Preload temperature of dual-mode controller
Q	Heat transferred to the system from the surrounding
Q_{exo}	Exothermic heat released
Q_j	Energy inside the jacket
Q_r	Energy inside the reactor
r	Radius of reactor
R	Reaction rate
R_i	Reaction rate of Reaction i
t	Time

T_c	Fluid temperature
TD-1	Time period setting of dual-mode controller 1
TD-2	Time period setting of dual-mode controller 2
T_j	Jacket temperature
T_r	Reactor temperature
T_{ref}	Reference temperature
U	Internal energy
U_r	Heat transfer coefficient between reactor and jacket
V	Volumetric holdup of the reactor contents
V_j	Jacket volume
W	Work done by the system on the surrounding
w_{est}	Estimated reaction parameter
W_r	Total weight of reactor contents
x	Control variable for GMC
x_{est}	Estimated reaction parameter
x^{sp}	Reference value for GMC
y_{est}	Estimated reaction parameter
z_{est}	Estimated reaction parameter

CHAPTER 1

INTRODUCTION

1.1 Overview of Exothermic Batch Process

The manufacturing process of chemical industries can be divided into two operation modes, namely continuous and batch. Both operation modes can be distinguished by looking at the charging and discharging manner of the reactor. For continuous operation mode, the reactor is charged and discharged continuously whereas, for batch operation mode, raw materials are initially charged into the reactor for a certain period to transform to other substances or products. This period is called as batch cycle time. The process will be repeated after the previous batch completed.

In the chemical industries, batch operation mode is preferable than continuous operation mode in producing high value-added products in small-volume, such as pharmaceuticals, agrochemicals, polymers, fine-chemicals, and other specialty chemicals. The batch operation mode has shown several advantages in chemical manufacturing. Firstly, batch operation mode is flexible to produce various products using the same plant equipments. Secondly, this operation mode is easier to scale-up from laboratory experiment to industrial manufacturing. Lastly, high risk reactions are easy to handle using the batch operation mode. Due to these advantages, the batch process has received foremost attention from researchers recently in optimising the batch productivity (Henini *et al*., 2011; Tan *et al*., 2011a; Zhang *et al*. 2012).

Generally, chemical reactions can be classified as either exothermic or endothermic. For exothermic, heat is released during the reaction, whereas for the endothermic, the heat of the environment is consumed during the reaction. Hence, exothermic reaction is more dangerous than the endothermic reaction because it will release unpredictable heat to the environment. Therefore, exothermic batch process is selected as the plant for this work.

In the normal circumstance of the exothermic batch process, a preheating may be needed for heating up the reactor in order to accelerate the reaction rate, hence reducing the overall batch cycle time. However, a large amount of heat is rapidly produced during the process which will further increase the reaction rate. To deal with this, a reliable cooling system is greatly needed to remove the generated heat. Although products manufactured using batch process are highly diverse, as discussed previously, they share the common aim of optimising the desired product while minimising the waste, because raw materials are usually very expensive. Therefore, coherence between the heating and cooling is a critical issue in order to have an effective control to optimise the batch productivity within a minimum batch cycle time. If the control system is not reliable, the reaction may become violent, or often known as thermal runaway, and will pose significant safety issue to the plant personnel and the community (Chen *et al.*, 2012).

1.2 Overview of Control Systems for Exothermic Batch Process

In order to achieve the process objective as well as to avoid the thermal runaway condition, it is vital to develop a reliable controller to control the process. However, due to the inherent dynamic behaviour and highly nonlinear characteristics of the exothermic batch process, the development of the control system becomes a challenging task for the control engineers. Since the temperature is the main factor contributing to the thermal runaway situation, the control system of the exothermic batch process basically is the issue of monitoring the process temperature.

Traditionally, process control of exothermic batch reactor is manually operated by human operator, for example dual mode controller (DMC). However, this method is highly depending on the expertise and knowledge of the operator in order to arrange the heating/cooling sequence, as well as the proportional-integral-derivative controller (PID) parameters tuning. Thus, optimum and consistent performances are rarely obtained because human expertise is usually perishable and unpredictable (Nisenfeld, 1996). From the economic point of view, human expertise is also usually very expensive. Today, advances in computer technology have urged the industries to employ the new technology in the control system.

Hence, various advanced control strategies are developed recently in order to reduce the dependency on the human expertise.

In general, the advanced control strategies can be divided into two major groups, namely predictive approach, such as model predictive control (MPC) and extended Kalman filter (EKF), and artificial intelligent approach, for example artificial neural network (ANN). The predictive approaches and ANN are used to predict the process behaviour and tune the parameters of slave controller, such as DMC. In order to have a better estimation about the process behaviour, these approaches need a huge batch of data to tune its parameters. This is a very difficult and complex task.

Therefore, genetic algorithm (GA) is proposed in this thesis to control and optimise the exothermic batch process because this approach is proven to be a guaranteed approach that can solve optimisation problem through the evolutionary process (Gosselin *et al*., 2009). The performance of GA is improved by introducing an adaptive fitness function so that it is able to predict the process behaviour and determine the suitable control actions to increase the production yield.

1.3 Scope of Work

This research is focusing on developing a reliable control system using GA for the exothermic batch process control and optimisation, as well as to avoid the thermal runaway condition. Various conditions which may cause the violent reactions are taken into account, such as insufficient cooling system, excessive heating, improper charging, and lack of understanding on the reaction chemistry. The efficiency and the robustness of the developed algorithm are also evaluated. This work starts with the review of the control and optimisation systems that have been developed in the past. The review provides the fundamental understanding of the exothermic batch process characteristics and relevant past research in this field. Referring to the basic fundamental laws of physics and chemistry, the exothermic batch process is modelled and simulated in MATLAB m-file. The GA is developed to control the exothermic batch process based on the predetermined optimal reference profile, and its effectiveness in controlling the process is investigated. Finally, the developed GA is evaluated to optimise the batch productivity.

1.4 Research Objectives

The objective of this research is to control and optimise the production of the desired product while minimising the waste production for an exothermic batch process. GA is proposed in this study, and the developed algorithm is applied to the exothermic batch process model to investigate its effectiveness and robustness. The research objective can be achieved through the following efforts:

1.4.1 To Model and Simulate the Exothermic Batch Process

The characteristics of the exothermic batch process are reviewed in order to have a comprehensive understanding on its behaviour. The mathematical modelling of the exothermic batch process is derived based on the fundamental theories of physics and chemistry. The process parameters, such as heat transfer rate and reaction heat, are obtained from a benchmark exothermic batch model. These parameters are used to describe the process characteristics at open-loop and closed-loop behaviours. Using the derived mathematical equations, the model is written in MATLAB m-file. In addition, a conventional DMC is also developed to test the process model, as well as to be used for the comparison with the proposed controller.

1.4.2 To Design and Develop the Genetic Algorithm

GA is selected as the controller to control and optimise the exothermic batch process. To enhance the robustness of the proposed algorithm, it is designed to manipulate multivariable (jacket inlet fluid temperature and flow rate). The conventional DMC applies preset settings which lead to less robustness in coping with unpredictable disturbance. To initiate the operation, the proposed GA will explore all the potential solutions (a combination of fluid temperature and flow rate), in order to determine a suitable combination for the instantaneous situation through its evolutionary ability. Lastly, the performance of the developed GA is observed.