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Development of PARS-EX pilot plant to study control strategies

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ABSTRACT

A PARtially Simulated EXothermic chemical reactor (PARS-EX) pilot plant is developed in this work to carry out and evaluate various conventional and advanced control strategies. In this reactor, the heat generated from the assumed exothermic reaction was simulated through the use of a controlled steam flow rate into the reactor. Since there is no actual reaction involved, the system is defined as a 'partially simulated' reactor. The temperature of the reactor was regulated by an external plate heat exchanger that both cools the process fluid and recycles it back into the reactor. A software interface was also developed to exchange real online data and implement the various control strategies. The advanced control strategies used to control the temperature of the reactor in this work are the neural network-based controllers, which overcome the hassle in periodically tuning conventional controllers. An adaptive method is also incorporated to cater for changes in the process conditions. Tests involving set point tracking and various external and internal disturbance changes were carried out to evaluate and demonstrate the robustness of the neural network-based controllers on the PARS-EX plant. For all of the realistic online cases studied, the neural network-based controllers exhibit better control results compared to the conventional controllers.

1. Introduction

Chemical reactors are used in many chemical, pharmaceutical and petrochemical processes, and temperature control is often a critical aspect of reactor operations. A reliable reactor containing an efficient temperature control system will contribute to the high quality of the final product. Reactors are usually equipped with external jackets or internal heat exchangers to remove excess unwanted heat energy that results from an exothermic reaction system. Coolant flow rates, typically water, into the jacket or heat exchanger are usually controlled using conventional feedback control strategies. Integrating conventional linear controllers has posed unique challenges when dealing with nonlinear reactor behavior (Chan, Leong, & Lin, 1995; Gerardo, Mihir Sen, Yang, & Rodney, 2001; Nikravesh, Farell, & Stanford, 2000). Hence, other advanced nonlinear methods have been investigated for controlling these reactors.

Recently, model-based control strategies such as predictive control and internal model control have been demonstrated using neural network models to control various chemical processes (Awais, 2005; Azwar, Hussain, & Ramachandran, 2006; Braake, te Hubert, van Can Eric, Jacquelien, & Verbruggen, 1998; Wachira, Piyanuch, Amornchai, Paisan, & Hussain, 2005; Yu & Gomm, 2003). These processes include many important chemical processes such as the petrochemical, pharmaceutical and food industries that play a vital role to the development of process industries (Hussain, 1999; Lennox, Montaque, Frith, Gent, & Bevan, 2001).

Neural network models have also been used and applied to various engineering areas for system identification (Nougues, Pan, Velo, & Puigjaner, 2000; Pham & Oh, 1999; Radhakrishnan & Mohamed, 2000; Saha, Shoib, & Kamruzzaman, 1998). Several researchers have investigated optimization studies utilizing neural networks to estimate process parameters that are difficult to measure in chemical processes (Aziz, Hussain, & Mujtaba, 2000; Mujtaba, Aziz, & Hussain, 2006; Mujtaba & Hussain, 1998). A more comprehensive review of neural network applications is available in the work by Hussain (1999), Hussain and Kershenbaum (2000) and Lennox et al. (2001). However, these researchers only considered the simulation case studies that lack experimental validation. Among the limited online applications of neural networks in chemical engineering processes are the application of neural network to model the temperature profile and behavior of an exothermic polymerization process (Chiaki & Jinyoung, 2002) and online neural network-based temperature control of a 16-l batch chemical reactor pilot plant using the highly exothermic reaction between thiosulfate and peroxide

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Nomenclature

F	flow rate (l/h)
V	volumetric (l)
C_{af}	feed concentration (mol/l)
C_a	reactant concentration (mol/l)
k	sampling instant at kth
k_o	pre-exponential factor (per h)
k_1	reaction rate constant (per h)
$(-\Delta H)$	heat of reaction (exothermic) (kcal/mol)
E	activation energy (kcal/h)
R	ideal gas constant
T	reactor temperature (K)
T_C	coolant jacket temperature (K)
UA	overall heat transfer coefficient (kcal/h K)
C_p	specific heat of water
ρ	density of water

Superscripts

Setp	set point
Gen	generated

(Florence, Marie-Veronique, Michel, & Gilbert, 2002). Neural network models have been primarily used in these applications because of their good performance in mapping arbitrary input-output relations and their capability to interpolate between given known operating points for nonlinear systems.

This work focuses on the development of an experimental, partially simulated exothermic pilot plant reactor to test various conventional and neural network-based control strategies. The word ‘partially simulated’ is used as there is no actual chemical reaction taking place in the reactor. Hence, this offers a cost effective method in testing various online control strategies within a reactor system (Cho, Edgar, & Lee, 2008; Hussain & Kershenbaum, 2000; Kershenbaum & Kittisupakorn, 1994). This system consists of a continuous stirred tank reactor (CSTR) coupled to a plate heat exchanger for cooling. Additionally, a pipe recycles the process fluid to enhance proper temperature distribution within the system. An exothermic first order chemical reaction, $A \rightarrow B$, is experimentally simulated in the reactor. The process mass and energy balances are used to derive the simulated reactant concentration and the heat generated in the reaction. The heat is then converted into equivalent steam flow rate that is supplied into the reactor, which simulates exothermic reactions. This is carried out online by calculating the amount of dry and saturated steam delivered from the main boiler into the reactor via a coil tube, to simulate the heat generated by the chemical reaction of interest. Since no actual reaction is involved, the reaction system is defined as a ‘partially simulated’.

This experimental setup system offers several advantages over the actual system, which uses real reactants. Firstly, the system is flexible, easily configured, comparatively safe and economical to operate. Secondly, it is capable of handling exothermic reactions with various kinetic mechanisms other than the first order reaction kinetics considered here. These can be carried out without the added concern of using dangerous chemicals that can also be expensive. Thirdly, the system also acts as a useful educational experimental system that is incorporated with a heat exchanger, flow transmitter, control valves etc. The experiment can factor in introduction of immeasurable and random disturbances, model mismatches and other real industrial limitations that usually are not considered in a simulation study. Finally, the safety and relatively simplicity of this system allows researchers to evaluate various advanced control and estimation algorithms under realistic industrial conditions. Reactors are important to the chemical industry, but experimental testing is both expensive and leads to environmental and safety hazards This pilot plant can be regarded as a reactor simulator that integrates all aspects of realistic industrial operations, which are important for student training and for control strategy testing. Using this proposed pilot plant, the cost of operation, maintenance and safety are significantly reduced as steam and water make up the inputs for the experimental reactor setup.

This paper is arranged as follows. After the Introduction section, The pilot plant used and reactor model is described. Then, two control strategies based on the inverse neural network model are elaborated and implemented. Online implementation for reactor temperature control, which involves Set point tracking and disturbance rejection case studies with the coolant jacket temperature as the manipulated variable, are then presented. This is followed by the Discussion and conclusion section.

2. The pilot plant

2.1. Process description and materials of construction

The constructed pilot plant consists of two main units: a continuous well-stirred reactor with an operating volume of 160 l and a plate heat exchanger unit, pictured in Fig. 1a, and its process schematic diagram (Fig. 1b). The reactor is charged and continuously with feed water. The feed water flow rate is controlled by a control valve and measured with a flow meter. The process fluid from the reactor is pumped through a plate heat exchanger and recycled back into the reactor. Changing the temperature of the recycled process fluid, which acts as the coolant jacket, regulates the average temperature in the reactor. The average temperature is taken as the average of three temperature sensors that are situated at different locations within the reactor. Cooling through the heat exchanger is controlled the supplying fresh water that is pumped through the heat exchanger. The reactor water level is monitored by a level transmitter and is regulated by manipulation of the control valve in the outlet line of the reactor. To simulate the heat generated by the reaction, an equivalent amount of energy is supplied to the reactor from a known steam flow rate, which is regulated via a control valve. A calculation for this regulated steam flow rate is discussed in later sections.

The reactor was constructed from 316 stainless steel and is resistant to corrosion from contact with water from the condensing steam. The operating temperature was around 50 °C with a maximum temperature limit of 90 °C. A 316 stainless steel helical coil was fit inside the reactor to heat the system using the steam condensing within it. The inner diameter of the coil is 2.45 cm (1 in) and the length is 3.5 m. The steam enters the coil downward into the reactor and is removed as a condensate from the bottom of the reactor. The maximum operating pressure and temperature for the plate heat exchanger is 5 bar and 90 °C, respectively. The design specifications for the heat exchanger are shown in Table 1. All of the pipelines were insulated with one inch thick rock wool insulation and covered with a 0.5 mm thick aluminum plate.