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Performance analysis of three advanced controllers for polymerization batch reactor: An experimental investigation

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ABSTRACT

The performances of three advanced non-linear controllers are analyzed for the optimal set point tracking of styrene free radical polymerization (FRP) in batch reactors. The three controllers are the artificial neural network-based MPC (NN-MPC), the artificial fuzzy logic controller (FLC) as well as the generic model controller (GMC). A recently developed hybrid model (Hosen et al., 2011a. Asia-Pac. J. Chem. Eng. 6(2), 274) is utilized in the control study to design and tune the proposed controllers. The optimal minimum temperature profiles are determined using the Hamiltonian maximum principle. Different types of disturbances are introduced and applied to examine the stability of controller performance. The experimental studies revealed that the performance of the NN-MPC is superior to that of FLC and GMC.

Keywords: Model based controller; NN-MPC; FLC; GMC; Hybrid model; Polystyrene

1. Introduction

Polymerization reactions are complex and exothermic in nature, which leads to the nonlinear behavior of polymerization reactors (Hvala et al., 2011). Control of polymerization reactors to obtain high quality polymer products is still a challenging task for researchers due to the reactor's nonlinear character (Özkan et al., 2009).

The main problem in controlling the polymerization reaction variables are whether these variables can be measured, estimated, or can be measured with some time delay (Ghasem et al., 2007). One of the major difficulties encountered in polymerization reactor control is the lack of reliable online real time analytical data. Reactor temperature as an intermediate variable is relatively easier to measure than the polymer structure properties (Zeybek et al., 2006). Therefore, an optimal control policy is essential to infer the optimal profile of intermediate variables (reactor temperature) to produce the desirable polymer structural properties such as the mechanical stress (molecular average molecular weight, number average molecular weight, and number average chain length), melt viscosity, hardness and elastic modulus. (Kiparissides, 2006).

In recent years, nonlinear model-based controllers (Dougherty and Cooper, 2003) have become popular to control the polymerization reactor (Van Brempt et al., 2001). This popularity is due to their ability to capture the nonlinear dynamics of the process (Zhang, 2008; Shafiee et al., 2008; Yüce et al., 1999). Various nonlinear model-based control techniques such as MPC, NN-based controller and GMC have appeared in the literature (Özkan et al., 2009; Alipoor et al., 2009; Ekpo and Mujtaba, 2008; Seki et al., 2001; Ali et al., 2010; Hur et al., 2003). Among all model-based nonlinear controllers, MPC is particularly popular for the dynamic optimization and control of chemical reactors (Shafiee et al., 2008; Sui et al., 2008). A number of applications of MPC in the control of batch polymerization reactor temperature control are listed in Table 1. Neural networks (NNs) offer the ability

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Nomenclature

A [m^2]	heat transfer area
A_d [s^{-1}]	frequency factor for initiator decomposition
A_p, A_t [1/mol s]	frequency factor for propagation and termination
C_p [J/g K]	specific heat of reactor mixture
E_d, E_p, E_t [J/mol]	activation energy for decomposition, propagation and termination
f [–]	initiator efficiency
H [–]	Hamiltonian
ΔH [J/g K]	heat of reaction
I [mol/l]	initiator concentration
I_0 [mol/l]	initial initiator concentration
k_d [s^{-1}]	rate constant for decomposition
k_p, k_t [l/mol s]	rate constants for propagation and termination, respectively
k_{tc} [l/mol s]	termination by combination rate constant
M [mol/l]	monomer concentration
M_0 [mol/l]	initial monomer concentration
Q [W]	heater power
R [J/mol K]	gas constant
R_m [mol/s]	rate of polymerization
T_j [K]	jacket temperature
T [K]	reactor temperature
T_{sp} [K]	reactor temperature setpoint
t, t_f [s]	time and polymerization time
U [W/(m^2 K)]	average heat transfer coefficient
V [l]	reactor working volume
X [%]	monomer conversion
X_n [–]	number average chain length
μ_0 [mol/l]	zeroth moment of dead polymer
ρ [g/l]	density of reactor mixture

to produce nonlinear models of industrial systems owing to their ability to approximate nonlinear functions and learn through experimental data (Qin and Badgwell, 2003; Mujtaba et al., 2006; Günay and Yildirim, 2013; Grondin et al., 2013). Most of the nonlinear predictive control algorithms based on NNs imply the minimization of a cost function by using computational methods for obtaining the optimal command to be applied to the process. In a recent study, Salau et al. (2009) used MPC and a conventional PID to control the temperature of gas-phase polyethylene reactor.

Özkan et al. (2009) investigated the online temperature control of a cooling jacketed batch polystyrene (PS) polymerization reactor using GMC. They achieved the temperature control of the polymerization reactor experimentally and theoretically, and the control results are compared with the previously published literature work. Shafiee et al. (2008) applied nonlinear model predictive control (NMPC) based on a piecewise linear Wiener model to a polymerization reactor to control the reactor temperature. In another study, Karer et al. (2008) studied a self-adaptive predictive functional control algorithm as an approach to the control of the temperature in an exothermic batch reactor. Nagy et al. (2007) and Khaniki et al. (2007) also used nonlinear model predictive control (NMPC) for the set point tracking control of an industrial batch polymerization reactor.

Besides MPC, artificial intelligence (AI)-based modeling and control techniques offer flexible and powerful solutions to the dynamic optimization and control of polymerization reactors

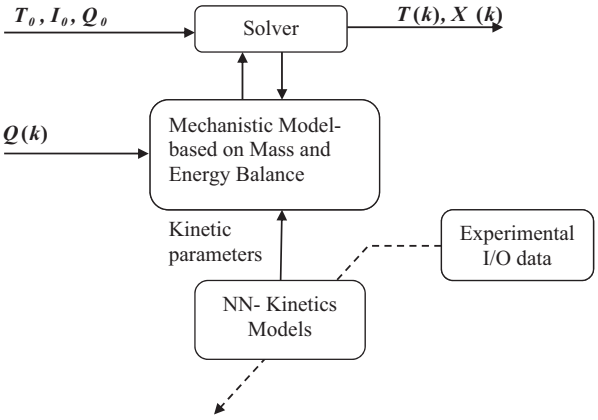

Fig. 1 – Hybrid model of polystyrene batch reactor (Hosen et al., 2011a). Based on initial conditions and operating parameters, and heater duty, this hybrid model directly predicts the reactor temperature as well as monomer conversion. The NN kinetics models are developed offline with experimental data and then the NN models are connected with the mechanistic (mathematical) model in series to construct the detailed PS reactor model.

(Stephanopoulos and Han, 1996). A number of applications of AI in the control of batch polymerization reactor temperature are listed in Table 1. The literature is rich in the application of different AI-based techniques to control polymerization reactors. It includes fuzzy logic controllers (Alipoor et al., 2009; Fileti et al., 2007; Çetinkaya et al., 2006; AltInten et al., 2006; Ghasem, 2006), neural network-based controllers (Zhang, 2008; Ekpo and Mujtaba, 2007, 2008) and genetic algorithm-based controllers (AltInten et al., 2006, 2008).

In this work, two artificial intelligence-based controllers (NN-MPC and FLC) and one nonlinear model-based controller (GMC) are developed and used to track the optimum set point of batch polymerization reactors. PS polymerization in a batch reactor is adopted for this study to check the efficiency of different advanced controllers.

2. Modeling of batch polystyrene reactor

Polystyrene product is produced by following a complex reaction mechanism in a batch reactor. The free radical polymerization process is commonly used to produce PS (Özkan et al., 2000). It is necessary to thoroughly understand the reaction mechanism and effective operating variables in order to develop a detailed model for the PS polymerization reactor. Researchers are still facing challenges to develop an effective model that leads to optimize the performance of a PS reactor (Herrera and Zhang, 2009).

Traditionally, polymerization reactors are modeled based on the mass and energy balance equations (Kiparissides, 1996). This conventional modeling technique usually suffers from high prediction errors (Konakom et al., 2008). A significant percentage of prediction errors arise from the kinetic model of polymerization reactor. This is due to the fact that the polymerization reactions are complex and researchers make many assumsptions or avoid some reactions in developing the kinetic model (Hosen et al., 2011a). In addition, the kinetic parameters for FRP are either partially known or completely unknown.

Considering the abovementioned issues, Hosen et al. (2011a) recently developed a hybrid model for PS batch reactor