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

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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 is whether these variables can be measured, estimated, or can be measured with some time delay (Chasem 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 Bremp 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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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; Güny and Yıldırım, 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, Kacer 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 (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 (Ali poor et al., 2009; Fileti et al., 2007; Çetinkaya et al., 2006; Altinten et al., 2006; Ghase m, 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 assumptions 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...
as represented schematically in Fig. 1. They developed offline nonlinear NN models to get kinetic parameters of this process. The kinetic parameters are the most effective state parameters for this process as process temperature variation directly depends on these parameters. Later, they combined these NN kinetics models with the first principle mechanistic model in series to get a detailed PS reactor model. They followed the methodology explained below to develop a hybrid model for the PS reactor (Hosen et al., 2011a).

(i) Firstly, implement the available conventional model and check the model prediction error with experimental data.

(ii) Conduct sensitivity analysis for the reactor temperature and kinetic parameters against reactor operating variables, and determine the effective operating parameters against kinetic parameters.

(iii) Conduct experiments to determine the reactor temperature profiles by varying the effective operation parameters. These include initial reactor temperature \(T_0\), initial initiator concentration \(I_0\) and initial heater duty or heater power \(Q_0\).

(iv) Parameter estimation analysis (using a nonlinear least square algorithm) is performed to estimate the kinetic parameters with the help of the conventional model (implemented in step i) and experimental data (collected in step iii). The estimated kinetic parameters involve frequency factors and activation energies for the decomposition, propagation, and termination reaction steps \((A_P, A_T, E_D, E_P, E_T)\).

(v) Develop three artificial neural network models to predict the kinetic parameters under the reactor operating conditions. Each NN model predicts the frequency factor \((A_P)\) and activation energy \((E_P)\) for the respective reaction steps where the initial reactor operating conditions \((T_0, I_0\), and \(Q_0\) are used as inputs for NN.

(vi) Finally, combine the trained NN-based kinetic model with the mechanistic model and validate the hybrid model with experimental data.

<table>
<thead>
<tr>
<th>Researcher</th>
<th>Type of research paper</th>
<th>System</th>
<th>Manipulated variable</th>
<th>Controller</th>
<th>Nature of research work</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ozkan et al. (2009)</td>
<td>Control</td>
<td>FRP of styrene in BR</td>
<td>Heater power</td>
<td>Applied Generic model control (GMC)</td>
<td>Simulation and experimental</td>
</tr>
<tr>
<td>Zhang (2006)</td>
<td>Control</td>
<td>FRP of MMA in BR</td>
<td>Heater power</td>
<td>Stacked neural network model</td>
<td>Simulation</td>
</tr>
<tr>
<td>Sui et al. (2008)</td>
<td>Control</td>
<td>FRP of styrene in BR</td>
<td>Jacket H&amp;C</td>
<td>Explicit moving horizon (model predictive) controller and an explicit moving horizon estimator</td>
<td>Simulation</td>
</tr>
<tr>
<td>Ekpo and Mujtaba (2008)</td>
<td>Control</td>
<td>FRP of MMA in BR</td>
<td>Heater power</td>
<td>GMC-NN and IMBC; the control vector parameterization (CVP) technique is used to pose the optimal control problem as an NLP problem, which is solved using SQP method within gPROMS</td>
<td>Simulation</td>
</tr>
<tr>
<td>Cho et al. (2008)</td>
<td>Control</td>
<td>General batch reactor</td>
<td>Jacket H&amp;C</td>
<td>Adaptive exact linearization control (AELC) with Sigma-point Kalman filter</td>
<td>Simulation</td>
</tr>
<tr>
<td>Beyer et al. (2008)</td>
<td>Control</td>
<td>FRP in BR-general</td>
<td>Jacket H&amp;C</td>
<td>Feedback nonlinear model predictive control</td>
<td>Simulation</td>
</tr>
<tr>
<td>Altitnten et al. (2008)</td>
<td>Control</td>
<td>FRP of styrene in BR</td>
<td>Heater power</td>
<td>Self-tuning PID control with GA</td>
<td>Experimental</td>
</tr>
<tr>
<td>Nagy et al. (2007)</td>
<td>Control</td>
<td>FRP of MMA in BR</td>
<td>Heater power</td>
<td>Feedback nonlinear model predictive control</td>
<td>Experimental</td>
</tr>
<tr>
<td>Khaniki et al. (2007)</td>
<td>Control</td>
<td>FRP of MMA in BR</td>
<td>Jacket H&amp;C</td>
<td>Applied globally linearizing Control (GLC) and MPC methods to control the temperature</td>
<td>Simulation</td>
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<tr>
<td>Fileti et al. (2007)</td>
<td>Control</td>
<td>FRP of MMA in BR</td>
<td>Coolant flow rate</td>
<td>PID-fuzzy logic controller</td>
<td>Simulation</td>
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<tr>
<td>Ekpo and Mujtaba (2007)</td>
<td>Control</td>
<td>FRP of styrene in BR</td>
<td>Heater power</td>
<td>Dual mode control with PID, GMC-NN and DIC</td>
<td>Simulation</td>
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<tr>
<td>Zeybek et al. (2006)</td>
<td>Control</td>
<td>FRP of styrene in BR</td>
<td>Heater power</td>
<td>Generalized delta rule (GDR) algorithm with generalized predictive control (GPC)</td>
<td>Experimental</td>
</tr>
<tr>
<td>Özkran et al. (2006)</td>
<td>Control</td>
<td>FRP of styrene in BR</td>
<td>Heater power</td>
<td>Nonlinear generalized predictive control; Levenberg-Marquardt algorithm is applied in the estimation of process parameters</td>
<td>Experimental</td>
</tr>
<tr>
<td>Çetinkaya et al. (2006)</td>
<td>Control</td>
<td>FRP of styrene in BR</td>
<td>Heater power</td>
<td>Fuzzy-relational models-dynamics matrix control (fuzzy-DMC) and compared with NLGPC</td>
<td>Experimental</td>
</tr>
<tr>
<td>Altitnten et al. (2006)</td>
<td>Control</td>
<td>FRP of styrene in BR</td>
<td>Heater power</td>
<td>Fuzzy control method with genetic algorithm</td>
<td>Experimental</td>
</tr>
</tbody>
</table>

FRP = free radical polymerization; MMA = methyl methacrylate; BR = batch reactor; H&C = heating and cooling.
Hosen et al. (2011a) validated the developed hybrid model with experimental data and claimed that this hybrid model prediction accuracy is superior to any other published PS reactor model. In the present work, this hybrid model is used to design and simulate the proposed controllers. For the control study purpose, the reactor temperature is chosen as a controlled variable while heater duty is employed as the manipulated variable. As can be seen in Fig. 1 that this hybrid model can predict T(t) with time for any value of Q(t). Thus, it is assumed that this model can represent the actual plant in the simulation study to check the controller’s performance.

3. Minimum time optimal temperature profile

Recently, researchers have successfully developed and used the optimal temperature profile to control the polymerization reactor to get the desired polymer product quality and quantity (Zeybek et al., 2004; Altipen et al., 2008; Özkan et al., 2001). In this work, the optimization problem involving minimum time optimal temperature policy has been formulated and solved for the PS batch reactor based on previous work (Zeybek et al., 2006; Sata, 2007). This optimal temperature profile is then used in the control studies.

The objective of the optimization problem is to generate an optimal temperature profile that leads to the desired final polymer product quality and quantity with minimum time (t_f). Here, the number average molecular weight (X_n) and the monomer conversion (X) indicate the polymer product quality and quantity, respectively. In order to minimize polymerization end-time, polymerization reactor temperature is employed as a control variable as the polymer product quality and quantity directly depend on reactor temperature. The target values for the optimization problem are chosen as X = 50% and X_n = 500 (Zeybek et al., 2006). The optimization problem is solved by using the Hamiltonian maximum principle (Ponnuswamy et al., 1987). Both algebraic and differential equations related to the PS reactor model are used in the optimization algorithm. The algebraic and differential equations are as follows (Zeybek et al., 2006):

The rate of initiation

\[ \frac{dI}{dt} = -k_{I}I \]  

(1)

The rate of monomer decomposition

\[ \frac{dM}{dt} = k_{p} \left( \frac{2k_{d}I}{k_{I}} \right)^{1/2} M = -k_{I}^{1/2}M \]  

(2)

The rate of dead polymer disperses (zeroth moment)

\[ \frac{dM_{0}}{dt} = k_{d}k_{I}I \]  

(3)

where

\[ k_{d} = A_{d} \exp \left( \frac{E_{d}}{RT} \right) \]  

(4)

\[ k_{1} = k_{p} \left( \frac{2k_{d}I}{k_{I}} \right)^{1/2} = A_{1} \exp \left( \frac{E_{1}}{RT} \right) \]  

(5)

\[ A_{1} = \left( \frac{2A_{d}}{A_{I}} \right)^{1/2} \]  

(6)

\[ E_{1} = \frac{2E_{p} + E_{d} - E_{t}}{2} \]  

(7)

\[ k_{d} = \frac{Q}{k_{I}} \left( 1 - \frac{u}{2} \right) \]  

(8)

\[ X = \frac{M_{0} - M}{M_{0}} \]  

(9)

\[ X_{n} = \frac{M_{0} - M}{\mu_{0}} \]  

(10)

The objective of the optimization problem is to calculate the minimum time optimal temperature policy to achieve a desired conversion, \( X_{d} \), and the number average of chain length, \( X_{n} \), for a given initial condition. According to the Hamiltonian principle, the following performance index needs to be minimized to achieve this goal (Ponnuswamy et al., 1987; Hapoglu et al., 2000):

\[ \min t_f = \max \left( -\int_{0}^{t_f} \frac{dt}{X} \right) \]  

(11)

In another form, the objective function can be expressed in terms of final time and weighted sum squares of difference of monomer concentration (M) and zeroth moment (\( \mu_0 \)) from their respective desired values (Ponnuswamy et al., 1987).

\[ J = \int_{0}^{t_f} \left( \frac{dt}{M} + w_{1} [M(t_f) - M_{d}]^{2} + w_{2} [\mu_{0}(t_f) - \mu_{ad}]^{2} \right) \]  

(12)

where \( w_{1} \) and \( w_{2} \) are the weighted function.

By applying the Hamiltonian maximum principle, Ponnuswamy et al. (1987) defined the relation of the objective function for minimum time optimal temperature policy with the Hamiltonian as follows

\[ H = -1 + p_{1} \frac{dp_{1}}{dM} + p_{2} \frac{dp_{2}}{dM} + p_{3} \frac{dp_{3}}{dM} \]  

(13)

or

\[ H = -1 - p_{1}k_{d}I - p_{2}k_{1}M_{I}^{1/2} + p_{3}k_{4}k_{d} \]  

(14)

where \( p_{1}, p_{2} \) and \( p_{3} \) are costate variables that satisfy the following equations.

\[ \frac{dp_{1}}{dt} = -\frac{dH}{dp_{1}} = p_{1}k_{d} + 0.5p_{2}k_{1}M_{I}^{-1/2} - p_{3}k_{4}k_{d} \]  

(15)

\[ \frac{dp_{2}}{dt} = -\frac{dH}{dp_{2}} = p_{2}k_{1}I^{1/2} \]  

(16)

\[ \frac{dp_{3}}{dt} = -\frac{dH}{dp_{3}} = 0 \]  

(17)

If \( T \) is unconstrained, the necessary conditions for optimality are written as

\[ H = 0; \quad \frac{dH}{dp_{1}} = 0; \quad \frac{d^{2}H}{dp_{1}^{2}} < 0 \]  

(18)

Hence, Eq. (14) can be written in the form of

\[ (p_{3}k_{4} - p_{1})k_{d}I - p_{2}k_{1}M_{I}^{1/2} - 1 = 0 \]  

(19)
Table 2—Reactor operating conditions and specifications.

<table>
<thead>
<tr>
<th>Name of the parameters</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific heat of reactor mixer (C_v)</td>
<td>1.96886</td>
<td>J/gK</td>
</tr>
<tr>
<td>Specific heat of jacketed water (C_p)</td>
<td>4.29</td>
<td>J/gK</td>
</tr>
<tr>
<td>Heat of reaction, (ΔH)</td>
<td>−57766.8</td>
<td>J/gK</td>
</tr>
<tr>
<td>Flow rate of jacketed water (m_i)</td>
<td>0.51</td>
<td>g/s</td>
</tr>
<tr>
<td>Gas constant (R)</td>
<td>8.314</td>
<td>J/mol K</td>
</tr>
<tr>
<td>Inlet temperature of jacketed water (T_i)</td>
<td>303.14</td>
<td>K</td>
</tr>
<tr>
<td>Average heat transfer coefficient (U)</td>
<td>55.1</td>
<td>W/(m² K)</td>
</tr>
<tr>
<td>Reactor working volume (V)</td>
<td>1.2</td>
<td>l</td>
</tr>
<tr>
<td>Reactor jacket volume (V_j)</td>
<td>1</td>
<td>l</td>
</tr>
<tr>
<td>Heat transfer area of reactor (A)</td>
<td>0.0533</td>
<td>m²</td>
</tr>
<tr>
<td>Density of jacketed water (ρ)</td>
<td>998.00</td>
<td>g/l</td>
</tr>
<tr>
<td>Density of reactor mixer (ρ)</td>
<td>983.73</td>
<td>g/l</td>
</tr>
</tbody>
</table>

\[
\frac{dH}{dT} = \left( \frac{p_1 E_k K_d^2 + p_2 E_k k_1 M_1^{1/2} - p_3 k_2 E_k K_d}{RT^2} \right)
\]

Therefore, both Eqs. (19) and (20) can be solved simultaneously to obtain the approximate optimal temperature

\[
T = \frac{-(E_1/R)}{\ln (E_d/A_1 p_2 M_1^{1/2} E_1 - E_d))}
\]

Fig. 2—Optimum temperature profiles with different initiator concentrations \([I_0 = 0.013 \text{ mol/l } (\text{--}), I_0 = 0.016 \text{ mol/l } (\text{---}), I_0 = 0.019 \text{ mol/l } (\text{--}))].

are connected to the computer via an analogue to digital (A/D) converter. Water as a coolant flows at a fixed rate through the jacket with an operated pump. The pump can be controlled by both manually and numerically.

In this study, the three main chemical components, styrene (99.9 mol%), toluene (99.9 mol%) and benzoyl peroxide (BPO) from Sigma-Aldrich, are used as monomer, solvent and initiator, respectively. The details of the experimental procedure can be found in elsewhere (Hosen et al., 2011a).

4. Batch polystyrene reactor system

The experimental system of the batch PS reactor used in this study is shown in Fig. 3. The apparatus consists of a 2.0 l jacketed glass reactor with a mechanical agitator and other utility items. The top of the reactor has four inlets for the agitator, heater, thermocouple and reflux condenser. The turbine agitator is used to stir the reactor mixture. The operating range of the agitator motor is 50 to 2000 rpm. An electric heater of 500 W is used to heat up the reactor mixture. A device called the triac module is used to control the heater power between 0 and 500 W as a system requirement. The heater is the manipulated variable for this system and the amount of heating power is determined by the controller used in this system. Nitrogen purges through the reactor mixture from the bottom of the reactor to provide an inert system for the reactions. A reflux condenser is used to collect the vaporized solvent that escapes with the nitrogen. One thermocouple is used to measure the reactor temperature. Another two thermocouples are positioned at the inlet and outlet of the cooling jacket to measure the coolant water temperature. The three thermocouples

5. Design of proposed controllers

In this work, two artificial intelligence-based controllers (NN-MPC and FLC) and one nonlinear model-based controller (GMC) are used to control the PS polymerization reactor. The previously developed hybrid model is used to determine the control parameters in a simulation study. Minimal time optimal temperature profiles are used as the setpoint reference trajectory. The controller’s performance criterion, integral absolute error (IAE) along with other performance metrics are used to check the efficiency of the controllers in simulation and experimental studies.

5.1. Artificial intelligence-based controllers

In recent year, neural networks are widely used to capture the nonlinear dynamic processes as the neural network directly
predicts the process output with high speed based on input without detailed process knowledge (Khosravi et al., 2010). This data-based modeling technique offers a great advantage for the model-based control algorithms. Computational loads as well as programming complexity for NNs are much easier than mathematical models (i.e. mathematical modeling involves a lot of differential and integral equations that lead to computational complexity and errors).

5.1.1. Neural network-based model predictive control

Time optimal control of the PS reactor provides temperature trajectories that can result in the production of polymers with desired properties. Model predictive control (MPC) is widely used to control the temperature of batch reactors (da Silva et al., 2012). Eaton and Rawlings (1992) defined MPC as a control scheme in which the control algorithm computes a manipulated variable profile that is optimized over a finite future time horizon, with an objective function subject to a number of plant model and constraint functions. The first move of this open-loop optimal manipulated variable profile is then implemented until a new plant measurement becomes available. Feedback is incorporated by using the new measurements to update the optimization problem.

The cost function for MPC to optimize the control signal for the PS reactor is defined as (Hosen et al., 2011b)

\[
\min_{u(k)} \left\{ f(k) = \sum_{p=1}^{N} \left| \sigma^* (k+p | k) - \sigma (k+p | k) \right|_M^2 + \sum_{q=0}^{N_u-1} \left| \Delta Q (k+q | k) \right|_A^2 \right\},
\]

subject to

\[
Q_{\min} \leq Q(k+p | k) \leq Q_{\max}, \quad p = 0, \ldots N_u - 1.
\]

\[
\Lambda Q_{\min} \leq \Delta Q(k+p | k) \leq \Lambda Q_{\max}, \quad p = 0, \ldots N_u - 1.
\]

\[
T_{\min} \leq \hat{T}(k+q | k) \leq T_{\max}, \quad q = 0, \ldots N
\]

where \( N \) and \( N_u \) denote as prediction horizon and control horizon, respectively. \( M_p \geq 0 \) and \( \Lambda_q > 0 \) are diagonal weighting matrices with dimensions \( n_y \times n_y \) and \( n_u \times n_u \), respectively, \( \sigma (k+p | k) \) denotes the model predicted outputs for the future sampling instant \( k+p \). The reference trajectory, \( \sigma^* (k+p | k) \), is typically assumed to be constant over the prediction horizon and equal to the desired set-point, i.e.

\[
\sigma^* (k+p | k) = \sigma^* (k).
\]

MPC greatly improves the system control accuracy and robustness. However, MPC based on linear process models may result in poor controller performance as most of the industrial chemical processes are nonlinear. Therefore, MPC based on nonlinear models is more desirable. NNs offer an alternative nonlinear model for MPC in industrial systems, owing to their particular abilities of approximating nonlinear functions and learning through example.

In this work, the NN is trained to capture the forward dynamics of the process. The NN model predicts the future plant output based on the previous plant inputs and outputs with some delay. The structure of NN plant model for MPC is represented by Fig. 4.

Experimental data of reactor temperature (plant output) for training the NN model are collected by varying the reactor heater power (manipulated variable). A total of 10,000 data
designing a good MPC controller it is important to specify the following controller parameters (Hosen et al., 2011b):

- Sampling interval
- Prediction and control horizons
- Constraints on the manipulated and output variables
- Weighting factors on input and output variables

In this work, a recently developed hybrid model (Hosen et al., 2011a) (as described in Section 2) is utilized to determine the sampling interval, prediction, and control horizon. The Marlin (1995) general tuning rule is used to determine the MPC sampling interval. As suggested by Sata (2007), a 3-s sampling interval is selected to satisfy Marlin’s general rule. The prediction and control horizon are determined by trial and error method. Closed loop simulations are carried out with optimum setpoint tracking using the hybrid model to optimize the prediction and control horizon. Different values of prediction and control horizon are employed in simulation and the NN-MPC performance is checked based on controller performance criterion, IAE. The simulation study shows that the prediction horizon of 24 sample intervals and the control horizon value of 4 sample intervals provide satisfactory control performance (see Hosen et al. (2011b) for more details). Design specifications of the NN-MPC controller are given in Table 4.

### 5.1.2. Fuzzy logic controller

The fuzzy logic controller (FLC) is one of the popular artificial intelligent-based controllers used in chemical plants (Altintent et al., 2003). It has the ability to handle multi-valued logic that allows intermediate values between conventional evaluations such as yes/no, positive/negative, true/false, and large/small. FLC can formulate mathematically the notion like positive or negative and quickly predicts the possible desired output.

There are three main parts to fuzzy logic operations, namely fuzzification, fuzzy processing and defuzzification as seen in Fig. 5. Fuzzification processes the input data to obtain the fuzzy input by the fuzzified the actual inputs. In fuzzy processing, predefined fuzzy rules produce the fuzzy outputs and defuzzification produces the actual controller output for a fuzzy output value. More details on fuzzy control and practical applications of this controller can be found elsewhere (Abdullah et al., 2011, Rahnamoun and Armaou, 2011).

In this work, the Mamdani-type inference is used to determine the fuzzy output (Cordón, 2011). The parameter values of the membership function in the FLC are listed in Table 5. The parameters $e$ and $ce$ denote the input parameters for FLC in terms of error $(T - T_{sp})$ and rate of error $[e(t) - e(t - 1)]$, respectively. The parameter ‘Q’ is the output. The fuzzy inference used in this work can be illustrated in Table 5.

### 5.2. Generic model controller

Generic model control (GMC) is an advanced model-based control strategy, which embeds a linear or nonlinear model of a system to compute an action in control (Samad et al., 2010).
The method uses only two tuning parameters. Furthermore, the nonlinear model does not need to be linearized as it utilizes the nonlinear model itself.

The GMC algorithm has been implemented recently as one of several advanced process control schemes in chemical engineering (Ekpo and Mujtaba, 2008). With the inclusion of nonlinear process models into the controller algorithm, GMC proves to be of an advantage as the process models can be used as they are without any linearization. It is relatively easy to employ the GMC algorithm in computer programming and a very effective response can be achieved by tuning only two GMC parameters, $K_1$ and $K_2$.

The GMC algorithm can be written in general form as follows (Ghasem et al., 2007):

$$\frac{dy}{dt} = K_1(y_{sp} - y) + K_2 \int (y_{sp} - y)dt$$  \hspace{1cm} (25)

where $y$ and $y_{sp}$ denote the current and setpoint value of control variables, respectively. The GMC parameters ($K_1$ and $K_2$) are tuned based on the tuning curve given by Lee and Sullivan (1988). The first expression in Eq. (25) drives the process back to steady state due to change in $dy/dt$. $K_2$ is tuned to make the process have a zero offset.

For the PS polymerization reactor system, Eq. (25) can be written as

$$\frac{dT}{dt} = K_1(T_{sp} - T) + K_2 \int (T_{sp} - T)dt$$  \hspace{1cm} (26)

An energy balance model of the reactor that reveals the relation between the controlled variable and the manipulated variable is important. Eq. (4) from the literature work of Hosen et al. (2011a) represents the energy balance equation for PS batch reactor.

$$\frac{dT}{dt} = \frac{Q + (-\Delta H) R_m V - UA (T - T_j)}{V \rho C_p}$$  \hspace{1cm} (27)

Combining Eqs. (26) and (27) gives $Q$ yields

$$Q = \left\{ K_1 (T_{sp} - T) + K_2 \int (T_{sp} - T)dt \right\} V \rho C_p + \frac{UA (T - T_j) - (-\Delta H) R_m V}{(-\Delta H) R_m V}$$  \hspace{1cm} (28)

The integral part of Eq. (28) has to be approximated by numerical integration (5th order Runge–Kutta integration). The kinetic model equations from Hosen et al. (2011a) are used to get the estimated value of heat released ($-\Delta H m$) from the reactions. Table 6 shows the parameters in GMC algorithm.

6. Results and discussion

In this study, three controllers are applied to investigate the accuracy and performance in controlling the batch reactor for PS production. The aim of the study is to implement these controllers in the regulation of the optimal temperature profile to produce the desirable (predetermined) polymer target, namely $X_n$, and end-of-reaction monomer conversion ($x$). Before the initiator is introduced into the reactor to initiate the polymerization, the reaction mixture consisting of monomer (styrene) and solvent (toluene) is maintained at a constant starting temperature of 364.4 K. This is the predetermined starting temperature of the optimal temperature profile at $t_0 = 0.016$ mol/l. The generation of the optimal temperature trajectory is explained previously in Section 3. The three controllers are employed.

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**Table 5 - Membership function for FLC.**

<table>
<thead>
<tr>
<th>Membership function for $e$</th>
<th>Left edge</th>
<th>Center</th>
<th>Right edge</th>
</tr>
</thead>
<tbody>
<tr>
<td>NS</td>
<td>Infinity</td>
<td>-2</td>
<td>1</td>
</tr>
<tr>
<td>ZR</td>
<td>-0.5</td>
<td>0</td>
<td>0.5</td>
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<tr>
<td>PS</td>
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<td>2</td>
</tr>
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<td>2</td>
<td>3.5</td>
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<td>PL</td>
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<td>4</td>
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<table>
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<th>Center</th>
<th>Right edge</th>
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<td>-0.1</td>
<td>0</td>
</tr>
<tr>
<td>ZR</td>
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<td>0</td>
<td>0.05</td>
</tr>
<tr>
<td>P</td>
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<td>Infinity</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Membership function for $T$</th>
<th>Left edge</th>
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<th>Right edge</th>
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<tbody>
<tr>
<td>Z</td>
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</tr>
<tr>
<td>H1</td>
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<td>40</td>
<td>60</td>
</tr>
<tr>
<td>H2</td>
<td>40</td>
<td>60</td>
<td>80</td>
</tr>
<tr>
<td>H3</td>
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<tr>
<td>H4</td>
<td>80</td>
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<td>H5</td>
<td>200</td>
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<td>400</td>
</tr>
<tr>
<td>H6</td>
<td>280</td>
<td>380</td>
<td>Infinity</td>
</tr>
</tbody>
</table>

$N$ = negative; $NS$ = negatively small; $ZR/Z = zero$; $P$ = positive; $PS$ = positively small; $PM$ = positively medium; $PL$ = positively large; $H(i) = intensity$ of heat, where $i = 1, 2, \ldots, 6$. 

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**Fig. 5 – Operation of a fuzzy controller.**
by manipulating the heater power to control the reactor temperature. The proposed controllers are tested with two study cases: the optimal tracking of setpoint and disturbance rejection study with the optimal tracking of setpoint.

6.1. **Online optimal control of polystyrene reactor**

In the present work, concentrations of 0.016 and 6.089 mol/l for initiator and monomer loading are chosen to produce the desired target as described in Section 3 (X = 50% and X_n = 500). Firstly, the NN-based MPC controller is investigated in real-time to track the optimal setpoint trajectory. The experimental results of optimal setpoint tracking for PS polymerization using NN-MPC are shown in Fig. 6. When the initiator is introduced to the reactor, the reactor temperature decreased suddenly and fell below the setpoint at nearly 1 K. This is because the initiator (at room temperature) is added to the reactor while the reactor temperature is at approximately 364.4 K. The MPC controller immediately takes action by increasing the heater power (Q) to level up the reactor temperature as setpoint, resulting in maximum overshoot of 0.5 K. Later, the temperature decays, decreasing in an oscillatory manner within 730 s. From this point onwards, the NN-MPC performance is good in terms of offset, overshoot and undershoot. However, a small oscillation can be observed throughout the batch operation. Fig. 6 also shows the transient response of the manipulating variable, heater power. The regulation is smooth. It is worth mentioning that the heater regulation is initially at Q = 150 W and it increases gradually at approximately 200 W at the end of the batch run.

The same initial operating condition is applied for the experimental study of FLC to control the PS polymerization reactor. Fig. 7 shows the experimental results of optimal setpoint tracking for FLC. The overall performance of the FLC is good to track the optimal setpoint. However, FLC took more time to come back to the setpoint after the initiator loading disturbance occurred. The manipulated variable (Q) also oscillates significantly.

Fig. 8 depicts the setpoint tracking performance of GMC controller. As can be seen in Fig. 8, the reactor temperature immediately dropped by 2 K when the initiator added into the reactor to initiate the reactions. This is because the initiator temperature is lower than the reactor steady state temperature. The GMC controller takes it as a disturbance and increases the value of manipulated variable (Q), which reaches a peak value at approximately 220 W. This extra effort of the controller increases the control variable, exceeding the setpoint value, and a maximum overshoot (by 2 ◦ K) can be observed in the GMC tracking. However, the controller is able to achieve stable setpoint tracking at the time instance of 1900 s. At this time, the controller closely tracks the setpoint profile without any offset. As seen in Fig. 8, the controller produces a smooth manipulation with minimum oscillation.

6.2. **Optimal tracking with disturbance**

Normal real operation of any chemical process always encounters disturbances due to existence of impurities, external conditions variation and changes of internal condition. In this investigation, two step disturbances are made in the process operation. Disturbances are made by increasing the values of the coolant flow rate and the inlet jacket temperature at a certain time from their normal operating values. The first and second step disturbances are introduced at time 2500 and 4500 s, respectively in the same experimental run. In the first disturbance, the coolant flow rate is increased from 60 to 100 ml/s at time 2500 s. Fig. 9 shows that the NN-MPC controller tracks the trajectory without significant overshoot or

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**Table 6 – Important parameters and control variables of GMC controller.**

<table>
<thead>
<tr>
<th>α∆H(J/mol)</th>
<th>V (l)</th>
<th>U (W/m² s)</th>
<th>A (m²)</th>
<th>ρ (g/l)</th>
<th>C_p (J/gK)</th>
<th>K_1</th>
<th>K_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>57766.8</td>
<td>1.2</td>
<td>55.1</td>
<td>0.053</td>
<td>983.73</td>
<td>1.96886</td>
<td>0.01</td>
<td>0.000012</td>
</tr>
</tbody>
</table>

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**Fig. 6 – Optimal setpoint tracking using NN-MPC.**
offset when the change of flow rate is made. There is a little oscillation of temperature in tracking the profile. Due to the increase of cooling water flow rate, the controller acts in such a way to remove the disturbance by increasing the heater output. This is due to the fact that increasing the flow rate enhances the heat transfer from the reactor mixture to the water jacket. This will reduce the temperature inside the reactor. These are also observed in Figs. 10 and 11 for setpoint tracking with disturbance using FLC and GMC, respectively. Another disturbance is introduced at the time of 4500 s where the inlet jacket temperature is increased from 303 to 323 K. In Figs. 9–11, it can be seen that the controllers act in such a way to eliminate the disturbance by reducing the amount of heat input to the reactor mixture and overshoot occurred when the disturbance is introduced. In comparison to the previous disturbance, the action of manipulated heater is more drastic. As can be seen from the figures, there is a sharp drop in the manipulated values.

6.3. Performance evaluation of NN-MPC with FLC & GMC

The polymerization reaction involves a complex reaction mechanism making the system nonlinear in nature. The aim
of this study is to achieve a better, smooth performance by using different advanced controllers. In this section, the experimental results of NN-MPC are compared with that of FLC and GMC.

As discussed in Section 6.1, Figs. 6–8 show the optimal setpoint tracking using NN-MPC, FLC and GMC, respectively. It can be seen in all of these figures, the reactor temperature immediately drops to 2–3 K from the setpoint when the initiator is added to initiate the polymerization. This is because the charging initiator is stored at a room temperature of 303 K. Consequently, the controllers act through manipulating the heater power to bring the temperature closer to the setpoint. However, it is observed that the controllers overreact causing a significant overshoot over the setpoint. The maximum overshoots are 0.5, 1 and 2 K for NN-MPC, FLC and GMC, respectively. The NN-MPC takes only 730 s to return back to setpoint from overshoot while FLC and GMC took about 1000 and 1900 s, respectively. More oscillations are observed for FLC while NN-MPC and GMC tracking the setpoint with little or without oscillation. Figs. 6–8 also depict the time evolution of heat input into the reactor mixture. Due to the large temperature difference in the initial stage, the manipulation of heater power increases tremendously until it reaches the maximum value at approximate 250 W. More oscillations are also observed in the action of the manipulated variable for FLC than the NN-MPC and the GMC.

Fig. 9 – Optimal tracking with disturbance rejection using NN-MPC.

Fig. 10 – Optimal tracking with disturbance rejection using FLC.
Figs. 9–11 depict the experimental results of NN-MPC, FLC and GMC control for disturbance rejection along the optimal trajectory. The same experimental procedure is followed to examine the controller’s stability with disturbance. The disturbances are introduced as discussed in the previous section. The polymerization begins when the reactor experiences a drop of temperature to 2 K. The three controllers adjusted the manipulated variable (by increasing the heater power) to reach the optimal setpoint. The first stable tracking is found at time 750 s for the NN-MPC while the FLC and the GMC took more time (1400 and 2000 s, respectively). The first disturbance is introduced at time 2500 s. Due to the impact of changing the cooling water flowrate, the temperature drops from the setpoint profile. In order to reject the disturbance, the controller tries to work up to the setpoint. After 400 s of the disturbance introduction, the NN-MPC controller is able to bring the temperature closer along the setpoint profile with little oscillation. The oscillation with offset (around 2 K) can be found for the FLC and the GMC and they have taken more time to come back the setpoint (approximately 1000 s).

At a time of 4500 s, the inlet jacket temperature is increased from its nominal temperature to introduce the second disturbance, and again the controllers acted to the response by decreasing the manipulated variable instantaneously as the reactor temperature increases with the increase of coolant temperature. The performance of the NN-MPC is better than the corresponding FLC and GMC in terms of oscillatory behavior, offset and stable setpoint tracking in this case as well. The significant oscillation is observed throughout the setpoint tracking with and without disturbance for the FLC. Table 7 shows the calculated control performance criteria in terms of maximum overshoot, average offset and settling time for setpoint tracking with disturbances. As can be seen in Table 7, the NN-MPC is able to reject the disturbance better than other controllers.

Besides the time-profile response analysis, comparison can also be made using quantitative and qualitative performance criteria. The results of the IAE and the integral square error (ISE) are taken as quantitative performance criteria and the target conversion and the number of average chain length are used as qualitative performance criteria for all controllers. The results are presented in Table 8. All the criteria investigated clearly show that the NN-MPC controller is superior to the FLC and GMC. Furthermore, NN-MPC controller is able to reject the disturbance better than the other two controllers in term of response after the disturbance introduction. It is noticed that the NN-MPC also demonstrates minor oscillations, especially at the time of startup and with smaller magnitude than in the FLC and GMC. Overall, the NN-MPC strategy secures superiority in term of the qualitative and quantitative criteria. In addition, the controller performance can be evaluated analytically. The $X_n$ value and polymer conversion are determined.

**Table 7** – Control performance criteria in terms of maximum overshoot, average offset and settling time.

<table>
<thead>
<tr>
<th>Controller</th>
<th>Maximum overshoot (K)</th>
<th>Average offset (K)</th>
<th>Settling time 1 (s)</th>
<th>Settling time 2 (s)</th>
<th>Settling time 3 (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NN-MPC</td>
<td>0.5</td>
<td>0.1</td>
<td>750</td>
<td>400</td>
<td>500</td>
</tr>
<tr>
<td>FLC</td>
<td>1.5</td>
<td>0.6</td>
<td>1400</td>
<td>1000</td>
<td>900</td>
</tr>
<tr>
<td>GMC</td>
<td>2.5</td>
<td>0.2</td>
<td>2000</td>
<td>1000</td>
<td>1400</td>
</tr>
</tbody>
</table>

**Settling time 1**: Stable setpoint tracking just after reaction start-up.

**Settling time 2**: Stable setpoint tracking after 1st disturbance.

**Settling time 3**: Stable setpoint tracking after 2nd disturbance.
at the end of polymerization. The quantitative and qualitative results for different controllers are presented in Table 8. As per these results, the NN-MPC control strategy also gives the nearest value of $X_0$ and conversion ($X$) target. In conclusion, the NN-MPC gives the best numerical results for setpoint tracking and the end use polymer quality. According to Table 8, a higher conversion (more than 50%) is achieved using the GMC. However, polymer quality (molecular weight) is much more important than conversion in this system. A higher conversion is not acceptable with polymer quality, because conversion can only be reached with the deviation of the optimum setpoint by the controller.

7. Conclusion

In this work, a simulation and an experimental investigation are performed for the temperature control in the batch solution polymerization of styrene. The polymerization reactor control is a challenging task as the polymerization reaction is complex and nonlinear in nature. Three advanced nonlinear controllers are designed and implemented in a real PS plant. The controllers used are NN-MPC, FLC and GMC. Due to the lack of available online sensors to measure the polymer properties, temperature is used to infer an objective of having the desired conversion and number average chain length ($X_o$). The proposed controllers are tested with various implementations including the optimal temperature batch recipe and process disturbance rejection. Two disturbances are introduced (changed operating parameters) in real time to check the stability of these controllers. The results of the NN-MPC are highlighted and compared to the other advanced controllers. The experimental results reveal that the NN-MPC is superior to track the optimal reactor temperature profile without noticeable overshoot as observed in the case of a FLC or GMC with and without disturbances. In conclusion, it is clear that the NN-MPC implemented in this work outperforms than other advanced controllers in terms of setpoint tracking and load rejection capabilities.

References
