

# Performance Analysis of Two Advanced Controllers for Polystyrene Polymerization in Batch Reactor

Mohammad Anwar Hosen, Abbas Khosravi, Saeid Nahavandi, Douglas Creighton and Mohd Azlan Hussain

**Abstract**—The performance of two advanced model based non-linear controllers is analyzed for the optimal setpoint tracking of free radical polymerization of styrene in batch reactors. Artificial neural network-based model predictive controller (NN-MPC) and generic model controller (GMC) are both applied for controlling the system. The recently developed hybrid model [1] as well as available literature models are utilized in the control study. The optimal minimum temperature profiles are determined based on Hamiltonian maximum principle. Different types of disturbances are artificially generated to examine the stability and robustness of the controllers. The experimental studies reveal that the performance of NN-MPC is superior over that of GMC.

**Index Terms**—Model based controller, NN-MPC, GMC, Hybrid model, Polystyrene

## I. INTRODUCTION

Polymerization reactions are exothermic in nature. The amount of heat released by the monomer to convert to polymer is considerable. Temperature variations in polymer process directly affect the quality of polymer products (i.e. physical properties and quality characteristics). Temperature control is, therefore, critical in the production of high quality polymers and specialty products of desired molecular structures [2].

In recent years, nonlinear model based controllers [3] as well as artificial intelligence-based controller have become [4] very popular to control the polymerization reactor because of the ability of these controllers to capture the nonlinear dynamics of the process [5, 6]. Various nonlinear process model based control techniques (MPC, NN based controller, GMC) have appeared in the literature [2, 4, 7]. However, most of these are limited to simulation studies [7].

In this work, two controllers, NN-MPC and GMC, are used to track the optimum setpoint of batch polymerization

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M. A. Hosen is with the CISR, Deakin University, Geelong Waurn Ponds, Australia (phone: +61 3 5227 1352; fax: +61 3 5227 1046; e-mail: a.hosen@research.deakin.edu.au).

A. Khosravi is with the CISR, Deakin University, Geelong Waurn Ponds, Australia (e-mail: abbas.khosravi@deakin.edu.au).

S. Nahavandi is with the CISR, Deakin University, Geelong Waurn Ponds, Australia (e-mail: saeid.nahavandi@deakin.edu.au).

D. Creighton is with the CISR, Deakin University, Geelong Waurn Ponds, Australia (e-mail: douglas.creighton@deakin.edu.au).

M. A. Hussain is with Chemical Engineering Department, University of Malaya, 50603 Kuala Lumpur, Malaysia (e-mail: mohd\_azlan@um.edu.my).

reactors. Styrene polymerization reaction adopted for this study.

The rest of this paper is organized as follows. In Section II, NN-MPC and GMC control strategies are developed and optimized the controller tuning parameters in simulation for close loop control of the polystyrene reactor system. Section III illustrates the real time control of polymerization reactor using NN-MPC and GMC. The controllers are tested with various implementations including the optimal temperature batch recipe and disturbance rejection. The quantitative and qualitative performance of the controllers are also describes in this section. Section IV concludes the work done in this article as well as finding of the present work

## II. CONTROLLER DESIGN

In this work, one artificial intelligence based controllers (NN-MPC) and one nonlinear model based controller (GMC) are used to control the polystyrene polymerization reactor. The developed hybrid model is used to determine the control parameters in a simulation study.

### A. Neural Networks based Model Predictive Control (NN-MPC)

Model predictive control (MPC) is widely used to control the temperature in batch reactors. Eaton and Rawlings (1992) [8] defined MPC as a control scheme in which the control algorithm computes a manipulated variable profile that optimizes an objective function over a finite future time horizon 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.

NN model is used in MPC as a nonlinear model [9]. The experimental data of the manipulated variable (heat load  $Q$ ) and plant output (reactor temperature  $T$ ) at  $t$  with two time delay units are used as inputs while the plant output reactor temperature at  $t+1$  is used as outputs for training the NN. The Levenberg–Marquardt method is used to train the NN based on a minimizing cost function. The mean square error (MSE) is used here as the cost function. It is expressed mathematically as:

$$\text{MSE} = \frac{1}{n} \sum_{k=1}^n (T_{\text{tg}}(k) - T_N(k))^2 \quad (1)$$

where  $n$  is the number of training data,  $T_{\text{tg}}$  is the target/desired reactor temperature and  $T_N$  is the NN output.

The design specifications for NN model considered in this study are given in Table I.

TABLE I  
DESIGN SPECIFICATIONS OF NN MODEL

No. of input nodes	6	
No. of hidden layer nodes	10	
No. of output nodes	1	
Total sample size	10000	
Training function	Levenberg-Marquardt Method	
	Sample size	Mean square error
Training data	5000	$5.36 \times 10^{-6}$
Testing data	2500	$4.13 \times 10^{-6}$
Validation	2500	$4.69 \times 10^{-6}$

In this work, the developed hybrid model is utilized to determine the NN-MPC parameters such as sampling interval and prediction and control horizon. Marlin [10] general rule is used to determine the sampling interval of MPC. The prediction and control horizons are determined by trial and error method [11]. The optimised parameters of the NN-MPC controller are given in Table II.

TABLE II  
DESIGN SPECIFICATION OF MPC

Prediction horizon ( $N_2$ )	24
Control horizon ( $N_u$ )	4
Control weight factor (M)	0.09
Move suppression factor( $\Lambda$ )	0.003
Minimization routine	Backtracking

### B. Generic Model Controller (GMC)

The GMC algorithm was implemented recently as one of the advanced process controllers in the field of chemical engineering [4]. It is relatively easy to employ the GMC algorithm and the desired response can be obtained by tuning only two parameters,  $K_1$  and  $K_2$ . Another great advantage of GMC is that the nonlinear model could be directly utilized in this controller. The GMC algorithm can be written in a general form as follows:

$$dy/dt = K_1(y_{sp} - y) + K_2 \int (y_{sp} - y) dt \quad (2)$$

where  $y$  is a current value of control variable and  $y_{sp}$  is a setpoint value of the control variable. Proper adjustment of the parameters  $K_1$  and  $K_2$  can be achieved based on the tuning curve given by Lee and Sullivan (1988). First expression in the Equation (2) 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.

Energy balance model gives the relationship between the controlled variable (temperature) and the manipulated variable ( $Q$ ). Therefore, assumption is made that all heat transferred occurs across the wall of the reactor. This gives the energy balance of the reactor mixture as

$$\frac{dT}{dt} = \frac{Q + (-\Delta H) R_m V - UA(T - T_j)}{V \rho C_p} \quad (3)$$

Replacing  $T$  by  $y$  and  $T_{sp}$  by  $y_{sp}$  in Equation (2) and combining Equation (2) and (3) to obtain  $Q$  lead to:

$$Q = \left\{ K_1 (T_{sp} - T) + K_2 \int_0^t (T_{sp} - T) dt \right\} V \rho C_p + UA(T - T_c) - (-\Delta H) R_m V \quad (4)$$

In order to estimate the heat released ( $-\Delta H \cdot R_m$ ), polystyrene process model Equations [1] are integrated and solved to give the estimated value. Table III shows the important parameters in GMC algorithm.

TABLE III  
IMPORTANT PARAMETERS AND CONTROL VARIABLES OF GMC CONTROLLER

$-\Delta H$ (J/mol)	V (ltr)	U (W/m <sup>2</sup> s)	A (m <sup>2</sup> )
57766.8	1.2	55.1	0.053
$\rho$ (g/ltr)	$C_p$ (J/gK)	$K_1$	$K_2$
983.73	1.96	0.01	0.000012

### III. RESULTS AND DISCUSSION

In this study, styrene, toluene and benzoyl peroxide are used as monomer, solvent, and initiator, respectively to produce polystyrene. A recently developed hybrid model [9] is used to design and simulate the studied controllers. Minimal time optimal temperature profiles are used as setpoint reference trajectory. The objective of optimization problem is to calculate the optimal temperature policy for a given initial initiator and monomer concentration that minimizes the reaction time,  $t_f$ , required to achieve a desired final monomer conversion,  $X_d$  (%) and number average chain length (NACL). The target value are chosen as  $X_d=50$  and NACL=500 to calculate optimal temperature profiles [5, 12, 13].

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

For experimental study, the concentration of 0.016 mol/l and 6.089 mol/l for initiator (benzoyl peroxide) and monomer (styrene) loading are chosen to produce the desired target of polystyrene product (i.e. 50% conversion and 500 NACL). The current chosen value of NACL is based on the commonly used optimal condition for control of polystyrene batch reactor [14, 15].

Before the initiator is introduced into the reactor for the polymerization to start, the reaction mixture consisting of monomer (styrene) and solvent (toluene) is maintained at a constant starting temperature of 364.4K. This is the predetermined starting temperature of the optimal temperature profile at  $I_0 = 0.016$  mol/ltr. The two controllers are employed by manipulating the heater to control the reactor temperature. The proposed controllers are tested with two cases: the optimal tracking of set-point, and disturbance rejection study with the optimal tracking of setpoint.

Firstly, NN-MPC and GMC controllers are investigated in real-time tracking the optimal trajectory. The

experimental results of optimal setpoint tracking of polystyrene polymerization using NN-MPC and GMC are shown in Fig. 1. As we can see from all figures, the reactor temperature immediately drops to 2-3K from setpoint when the initiator is added to initiate the polymerization. This is because the charging initiator is stored at room temperature of 303K. Consequently, the controllers acted through heater manipulation to bring the temperature closer to the setpoint. However, it is observed that controllers overreacted for this matter causing a significant overshoot over the setpoint. The maximum overshoots are 0.5K and 2K for NN-MPC and GMC respectively. The NN-MPC takes only 730sec to return back to the setpoint from overshoot while GMC takes about 1900 sec. The Fig. 1 also depicts the time evolution of heat input into the reactor mixture. Due to the large temperature difference in initial stage, the manipulation of heater increases tremendously until it reaches a highest limit of manipulated value at 200watt. More oscillation is also observed in the action of manipulated variable for GMC than NN-MPC.

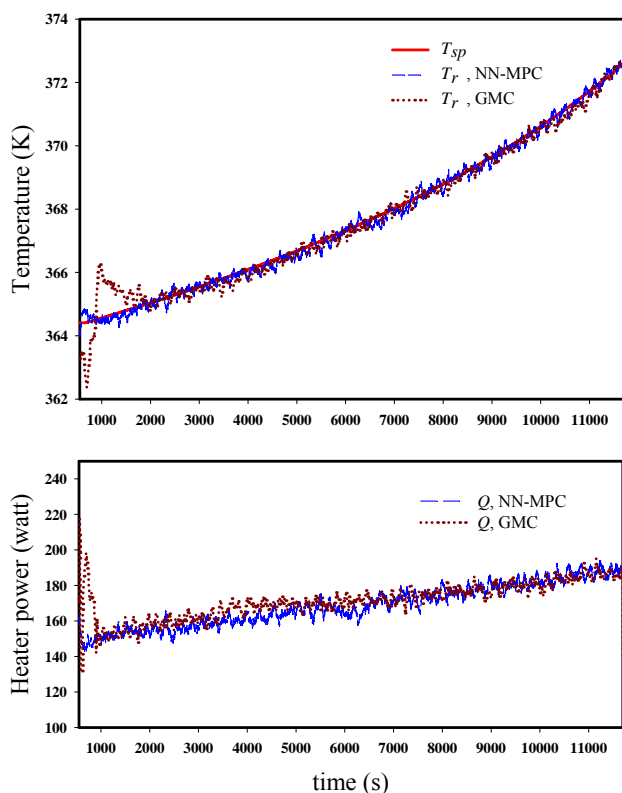


Fig. 1 Optimal setpoint tracking using NN-MPC and GMC

Normal operation of chemical processes always encounters disturbances such as impurities, external conditions' variation and changes of internal conditions. In this work, the process disturbances, namely the coolant flow rate and the inlet jacket temperature, are introduced by increasing the values from the nominal operation conditions at a certain time. The first and second disturbances are introduced at time 2500sec and 4500sec respectively in the same experimental run. In the first disturbance, the coolant flow rate is increased from 60 to 100ml/s at time 2500sec. Another disturbance is introduced at time 4500sec where the inlet jacket temperature is increased from 303 to 323K.

Fig. 2 depicts the experimental results of NN-MPC and GMC control for disturbance rejection along the optimal

trajectory. The same experimental procedure as before is followed to test the controller stability with disturbance. The polymerization began when the reactor experienced a drop of temperature to 2K. Both controllers adjust the manipulated variable (by increasing the heater power) to reach the optimal setpoint. The first stable tracking is found at time 750 sec for NN-MPC while GMC requires about 2000 sec to reach a stable setpoint tracking. The disturbance is introduced at time 2500 sec. 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. Definitely, this will reduce the temperature inside the reactor. In order to reject the disturbance, the controller tries to work up to the setpoint but later it ends up oscillating. After 400 sec of the disturbance introduction, the NN-MPC controller is able to bring the temperature closely along the profile with some oscillations. The huge oscillation with offset (around 2K) can be found for GMC and it takes more time to come back to the setpoint (near to 1000sec).

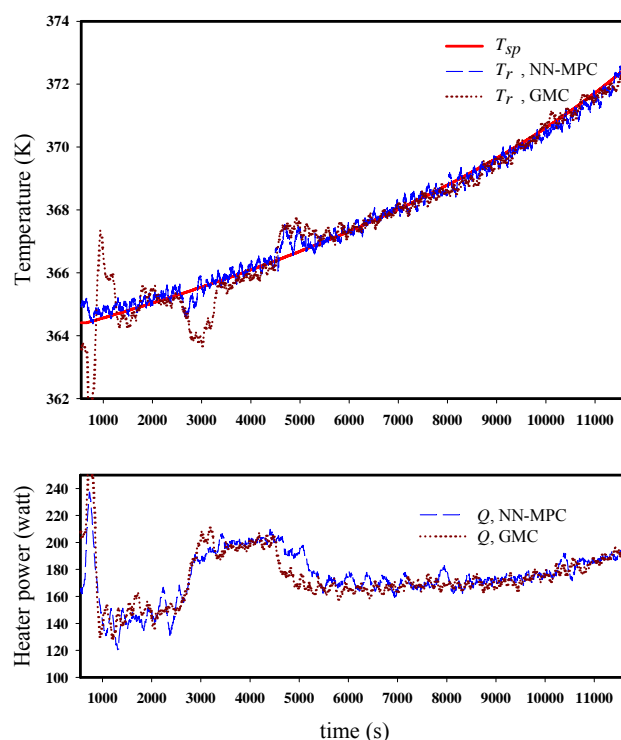


Fig. 2 Optimal tracking with disturbance rejection using GMC

At time,  $t=4500$  sec, the inlet jacket temperature is increased from its nominal temperature, and again the controller responds to this by decreasing the manipulated variable instantaneously because the reactor temperature rises with the increment of coolant temperature. In comparison to the previous disturbance, the action of manipulated heater is more drastic. As per Fig. 2, there is a sharp drop of manipulated values. The performance of NN-MPC is better than GMC in terms of oscillation behavior, offset, and stable tracking. Table IV shows the calculated control performance criteria in terms of maximum overshoot, average offset, and settling time for setpoint tracking with disturbances. Settling time 1 is the stable setpoint tracking just after reaction start-up. Settling time 2

is stable setpoint tracking after the 1<sup>st</sup> disturbance, and settling time 3 is stable setpoint tracking after the 2<sup>nd</sup> disturbance. According to results in Table IV, the NN-MPC is able to reject the disturbance better than GMC controller.

TABLE IV  
CONTROL PERFORMANCE CRITERIA IN TERMS OF  
MAXIMUM OVERSHOOT, AVERAGE OFFSET AND SETTLING  
TIME

Controller	Maximum overshoot (K)	Average offset (K)	Settling time1 (sec)	Settling time2 (sec)	Settling time3 (sec)
NN-MPC	0.5	0.1	750	400	500
GMC	2.5	0.2	2000	1000	1400

Besides the time-profile response analysis, comparison can also be made using quantitative and qualitative performance criteria. The results of the integral of absolute values of error (IAE) and the integral of square of the 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 V. All the criteria investigated clearly shows that NN-MPC controller is superior to the GMC. Furthermore, NN-MPC controller is able to reject the disturbance better than GMC controller in terms of response after the disturbance introduced. Though it is noticed that NN-MPC also demonstrates minor oscillation, it happens occasionally, especially at the time of start-up and with a smaller magnitude than the GMC. Overall, NN-MPC strategy secures superiority in terms of qualitative and quantitative criteria. In addition, the performance of controller can be evaluated analytically. The final properties of the polymer are determined at the end of polymerization. The results of monomer conversion and the number of average chain length (NACL) are presented in Table V. As per these, the NN-MPC control strategy also gives the nearest value of NACL and conversion (X) target. In conclusion, the NN-MPC gives the best numerical results for setpoint tracking and the final polymer quality. 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. Higher conversion is not acceptable with a poor polymer quality because conversion can only be reached with the deviation of optimum setpoint by the controller.

#### IV. CONCLUSION

In this work, simulation and online temperature control in a batch solution polymerization of styrene is presented. Temperature is used to infer an objective of having the desired conversion and number average chain length (NACL). The NN-MPC and GMC controllers are tested with various implementations including the optimal temperature batch recipe and disturbance rejection along the course of reaction. The results of the NN-MPC are highlighted and compared to the other advanced controller. The experimental results show that the NN-MPC is able to track the optimal reactor temperature profile efficiently and without noticeable overshoot. A better disturbance rejection is also shown by the NN-MPC compared to GMC. In conclusion, it is clear that the NN-MPC implemented in this

work outperforms GMC in terms of setpoint tracking and load rejection capabilities.

TABLE V  
QUANTITATIVE AND QUALITATIVE COMPARISON OF  
CONTROLLERS PERFORMANCE WITH DISTURBANCES

Case	Controller	Performance			
		NACL	Conversion (%)	IAE	ISE
Desired		500	50		
Optimum tracking without disturbance	NN-MPC	496	52.8	2513	2036
	GMC	473	54.2	3252	3552
Optimal Tracking with Disturbances (coolant flowrate & coolant tempt).	NN-MPC	482	53.2	3369	2647
	GMC	430	58	3846	3232

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