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APPLICATION OF MODEL PREDICTIVE CONTROL TO BATCH POLYMERIZATION REACTOR

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ABSTRACT

The absence of a stable operational state in polymerization reactors that operates in batches is factor that determine the need of a special control system. In this study, advanced control methodology is implemented for controlling the operation of a batch polymerization reactor for polystyrene production utilizing model predictive control. By utilizing a model of the polymerization process, the necessary operational conditions were determined for producing the polymer within the desired characteristics. The main control objective is to bring the reactor temperature to its target temperature as rapidly as possible with minimal temperature overshoot. Control performance for the proposed method is encouraging. It has been observed that temperature overshoot can be minimized by the proposed method with the use of both reactor and jacket energy balance for reactor temperature control.

Key words: control, MPC, polymerization, polystyrene**,** modeling.

RESUMEN

La ausencia de un estado operacional estable en reactores de polimerización es factor que induce la necesidad de un sistema especial de control. En este estudio se implementa una metodología para controlar la operación en un reactor de polimerización para la producción de poliestireno empleando un modelo predictivo de control. Las condiciones necesarias para operar fueron determinadas con el fin de producir el polímero dentro las características deseadas mediante la utilización de un modelo en el proceso de polimerización. El principal objetivo del control es llevar la temperatura del reactor hacia la temperatura necesaria, tan rápidamente como sea posible, sin sobrepasar los límites mínimos. La ejecución del control para el método propuesto mostró los buenos resultados. Se ha observado que el sobrepaso de la temperatura puede minimizarse mediante el método propuesto, el uso tanto del reactor como de un balance de la energía del mismo, para el control de la temperatura del reactor.

Palabras clave: control, polimerización, poliestireno, modelador.

INTRODUCTION

Non-linear identification techniques have been used for a long time and non-linear models are used in predictive control algorithms. Advanced control techniques need good identification data which cover the whole range of the process variable. In recent developments in modeling of non-linear dynamical systems such as neural networks open a new and stimulating road to black-box non-linear identification. Model-predictive control is a control scheme in which the controller determines

a control input profile that optimizes a given objective function on a time interval extending from the current time to the prediction horizon. Since the concept of model-predictive control was introduced to the industry by Richalet *et al*. (1978), various kinds of predictive controllers have been proposed in the literature whereas Soeterboek (1992) proposed the predictive controller of unified approach including the features of several well-known model-predictive controllers. Due to the complex reaction mechanism, the strong inherent nonlinearities, and the absence of steady state, the control of a batch polymerization process presents many problems. Furthermore, the model uncertainties are unavoidable as in most other chemical processes, and these features make the application of model-based controllers difficult. Adaptive control scheme is a potential solution and some studies have been performed in the domain of polymerization.

Several kinds of adaptive, nonlinear and model predictive control algorithms have been evaluated for the control of a batch polymerization reactor. Kiparissides and Shah (1983) applied adaptive control algorithms and a fixed gain PID controller to a batch polyvinyl chloride reactor, and carried out simulation studies. An adaptive pole-assignment controller was developed and corroborated experimentally by Tzouanas and Shah (1989). The performance of the generalized minimum variance controller was compared to that of the fixed gain PID controller. However, these adaptive pole-assignment controllers are difficult to be tuned in comparison to the model predictive controller though it may be reinterpreted as the model predictive controller with adaptive algorithm (Soeterboek, 1992). More recently, Soroush and Kravaris (1992) applied the globally linearizing control method, one of the nonlinear control algorithms, to a batch polymerization reactor and experimentally compared its performance with the conventional PID controller. Nevertheless, the nonlinear control algorithms are hard to be applied to the industrial processes because they still have critical problems such as lack of robustness and stability. Houston and Schork (1987) applied the adaptive model-predictive control algorithm to a semibatch polymerization reactor with a linear approximation whereas Kiparissides *et al*. (1990) used the long-range predictive control algorithm for the control of molecular weights in a batch polymerization reactor. These authors, however, confined their studies to the numerical simulation of the control system using mathematical model. Mendoza-Bustos *et al.* (1990) applied the robust adaptive control algorithm to the control of monomer conversion in a continuous stirred tank reactor (CSTR) in the presence of reactive impurities. In the present work, a control system for a batch polystyrene polymerization reactor (figure 1) was constructed by applying model predictive control. The controller performance was tested for nominal, sinusoidal, step change in reactor temperature set point, and optimum temperature profile to achieve 50% conversion of monomer and number average change length of 500.

Mathematical model

The following mathematical model of six nonlinear-state equations is based on mass and energy balances of the reactor mixture and the jacket as obtained from the literature (Ozken *et al*., 1998). The mass balance equations for the initiator and the monomer are:

$$\frac{dI}{dt} = -k_d I;\ I(0) = I_o \tag{1}$$

$$\frac{dM}{dt} = -k_p PM \quad M(0) = M_o \tag{2}$$

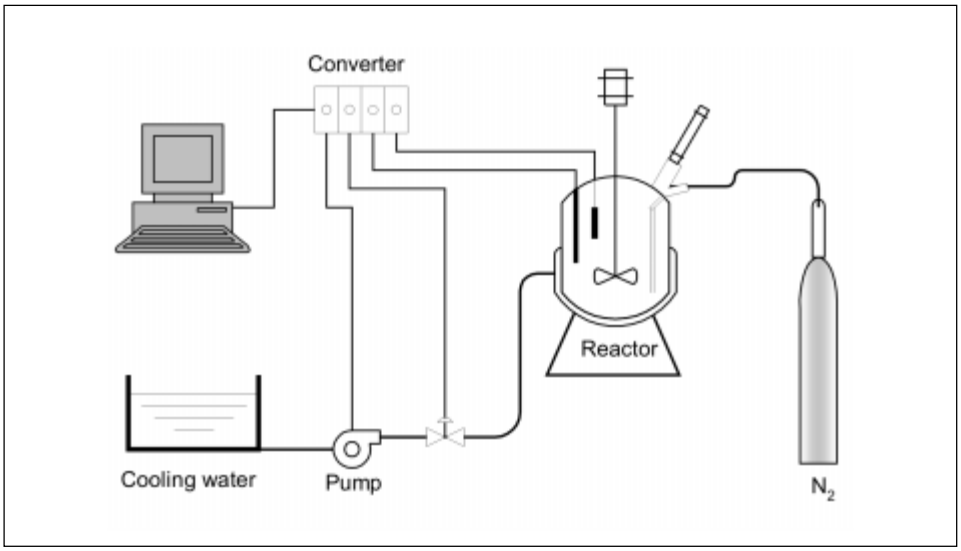

FIGURE 1. Schematic diagram of equipment of batch polymerization.

where, $P = \left(\frac{2f\,k_d I}{k_t}\right)^{0.5}$ *and* $k_t = k_{tc} + k_{td}$

The moment of dead polymer:

$$\frac{dq_o}{dt} = 2f\left(1 - \frac{\nu}{2}\right)k_d I \qquad (3)$$

where $\nu = k_{tc} \Big/ k_{td}$

$$\frac{dq_2}{dt} = (2 + \nu)\frac{k_p^2}{k_t} M^2 \qquad (4)$$

$$k_d = A_d \times \exp(-E_d / RT)$$
$$k_p = A_p \times \exp(-E_p / RT) \qquad (5)$$
$$k_t = A_t \times \exp(-E_t / RT)$$

Energy balances of the reactor and the jacket express the reactor dynamic.

$$\frac{dT}{dt} = \frac{q + (-\Delta H)R_m V - UA(T - Tc)}{V_\rho C_p} \qquad (6)$$

$$\frac{dTc_o}{dt} = \frac{M_c C_{P_c}(Tc_i - Tc_o) + UA\,(T - Tc)}{V_c \rho_c C_p} \qquad (7)$$

where, $R_m = \frac{dM}{dt}$; $Tc = \frac{Tc_i + Tc_o}{2}$

R_m is the overall rate of monomer.

The overall heat transfer coefficient,

$$U = U_0 - \alpha X \qquad (8)$$

The monomer conversion and the number average chain length are given respectively by,

$$X = \frac{M_o - M}{M_o} \qquad (9)$$

$$X_n = \frac{M_o - M}{q_o} \qquad (10)$$

Optimum temperature profile

The optimum temperature profile is the temperature under which the reactor should

produce a polymer product in a minimum time with 50% conversion and 500 number average chain lengths. The optimum profile was obtained using Hamiltonian maximum principle to the mathematical model of this process, detailed of the equations can be found elsewhere (Ponnuswamy et al., 1987).

By using Costate Hamiltonian and model equations, an equation for optimal temperature was obtained as

$$T = \frac{-(E_p + E_d/2 - E_t/2)/R}{\ln\left\{\dfrac{E_d}{p_2 I_0^{0.5} M A_p \left(\dfrac{2fA_d}{A_t}\right)^{0.5}\left(E_p - \dfrac{E_d}{2} - \dfrac{E_t}{2}\right)}\right\}} \qquad (11)$$

Figure 2 shows the computed optimal temperature profiles. The temperature profile depends on the initiator concentration, as the initiator concentration decreases, the temperature profile obtained is more close to isothermal case. To track these calculated optimal temperature profiles, controller used should act smoothly and precisely as much as possible.

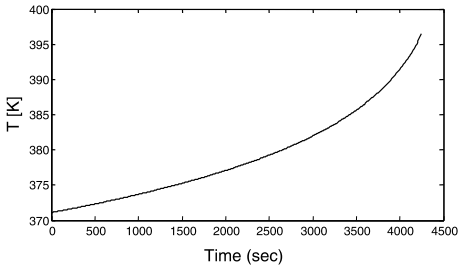

FIGURE 2. Optimum temperatures profile.

Model predictive control (MPC) scheme

In this section, a justification of the use of MPC controller is carried out and the main control algorithm is explained. For a set of present and future control moves $\Delta q(k)$, $\Delta q(k+1),\ldots, \Delta q(k+m-1)$ the future behavior of the process outputs $T(k+1|k)$, $T(k+1|k),\ldots, T(k+1|k)$ can be predicted over a horizon p. The m present and future control moves ($m \le p$) are computed. For a SISO plant, MPC determines its moves by solving the following optimization problem (formulated for the k^{th} sampling instant).

Table 1
Parameters and given conditions for styrene polymerization reactor

A_d (l/s)	2.6×10^{16}
A_P (l/s mol)	1.051×10^{7}
A_t (l/s mol)	1.255×10^{9}
C_p (J/mol K)	199.13
E_d (kJ/mol K)	143.161
E_P (kJ/mol K)	29.553
E_T (kJ/mol K)	7.0325
f	0.5
g	1
v	1
M_W (g/mol)	104.14
ρ (kg/m^3)	983.73
ΔH (kJ/kg)	57766.8
U_o (W/m^2 K)	55.1
V (l)	2
V_c (l)	2
D_T (m)	0.15

$$\underset{u_k,\ldots,u_{k+p-1}}{Min} \sum[w^y (r_{k+i} - \hat{y}_{k+i})2 + w^u (\Delta u_{k+i-1})^2] \qquad (12)$$

where $\Delta u_j = -u_{j-1}$ is the adjustment at sampling instant j, and w^y and w^u are non negative "weights"

Such that

$$\hat{y}_{k+i} = f(u_{k,\ldots,} u_{k+i-1}) \qquad (13)$$

Equation 13 is the *model* by which MPC predicts the controlled variable at instant $k+i$. In standard MPC, $\hat{y}_{k+i}$ is a linear function of the adjustments $u_k, \ldots, u_{k+i-1}$. The prediction $\hat{y}_{k+i}$ is a function of known and estimated disturbances, but these effects are constant, i.e. independent of the adjustments. They are implicit in equation (13).

Simulation method

The MPC GUI It is designed to help analyze and simulate the most common plant MPC controller and plant model combinations. It also provides a "worksheet" that help to keep track of your progress as you test different designs (Ricker *et al*., 1998). The GUI supports the following model types: Linear, either an LTI object (transfer function, state-space), or a step-response model and nonlinear, a SIMULINK block diagram. All standard linear MPC design options can be used. If the plant model is nonlinear, one can linearize it to design the controller, and then simulate linear MPC of the nonlinear plant. If the model is nonlinear, proper setting of initial conditions is very important.

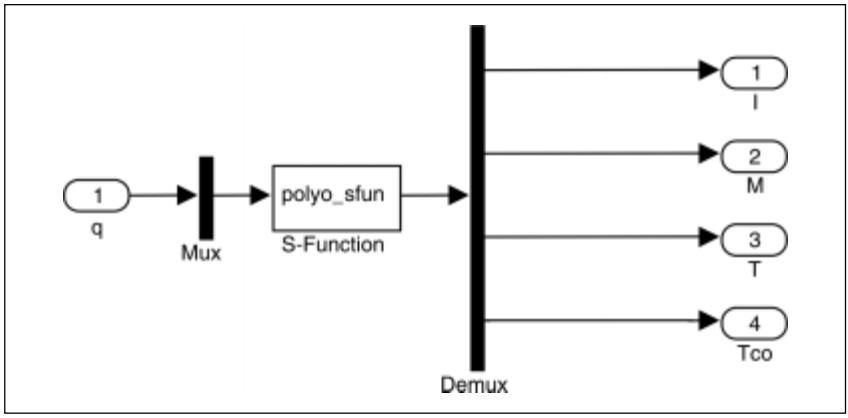

FIGURE 3. Simulink block diagram for styrene polymerization model (ps.mdl).

For cases to run a simulation with non-zero initial conditions, Simulink plant model must be used as shown in figure 3 of the present work. A function (more specifically, an S-function) file containing the model equations (algebraic and differential) to be integrated by SIMULINK, figure 3 shows the generated SIMULINK block diagram containing an S-function. When working with nonlinear models, if one observes unexpected behavior at the beginning of a simulation, the initial conditions are the first one should check. The final MPC GUI worksheet is shown in figure 4.

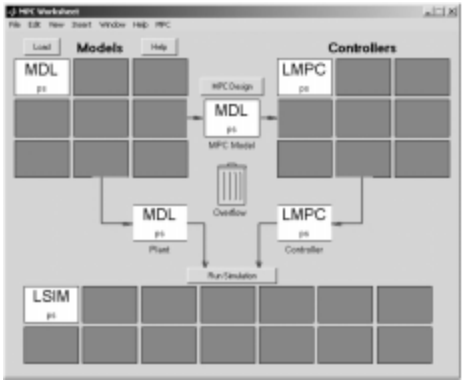

FIGURE 4. MPC GUI worksheet windows.

The initial values of input parameter are shown in table 2, After many trials the optimum MPC tuning parameters is shown in table 3.

Table 2
Initial values

Manipulated variable	State variable
q= 36 W (for nominal) q = 43 W (for sinusoidal)	I= 0.0126 mol/l M= 6.7 mol/l T=373 K T_c = 298 K

Table 3
Tuning parameters of MPC

Parameter	Value
P	7 block moves [115]
m	3
Weighting matrix of MV [Q]	[0.1]
Weighting matrix of CV [T]	[10000]

Results and discussion

By applying Hamiltonian maximum principle to the mathematical model of the process, optimum temperature, and initial initiator concentration were computed for different desired conversion and average number of molecular weight values. For this study, the desired conversion is 50% and the number average chain length of 500 was chosen to obtain the optimum polymer properties. Although 100% is required to obtain the polymer economically, it is very difficult to achieve this conversion and styrene does not exhibit an effective gel effect up to 50% conversion. To reach these desired values, optimal values for Temperature and initiator concentration were computed approximately as 100°C and 0.0126 mol/l, respectively. The optimal conditions used in the simulation studies are given in table 2. These calculated optimal temperature trajectories were used as set point changes during the polymerization. These optimal trajectories were shown in each figure that shows control results.

1. Nominal reactor temperature

At nominal conditions, the controller successfully sustained the reactor set point temperature at 373 K during the 4000 seconds of operation (figure 5). Initiator, monomer concentration, and jacketed temperature are dropping with time. Heat input to the reactor (q) increases with increasing time that is, to keep reactor temperature to its desired set point temperature (figure 6). The increase in the manipulated heat input to the reactor is due to decrease in reaction rate and hence decrease in the reaction heat released of the exothermal polymerization reaction. As a result, the MPC responses by increasing the heat supplied to the batch reactor to compensate the drop in the rate of released heat of reaction.

2. Tracking the sinusoidal changes in set point of the reaction temperature

In Figure 7 the reaction temperature set point is in sinusoidal form to trace the robustness and performance of the model predictive controller. It can be seen that the reactor temperature is sharply matching the reactor temperature set point. At the first 1000 seconds, as the temperature set point exponentially increased from 373 K to 375 K, the input heat to the batch reactor is almost constant since the rate of reaction is high in this region, and therefore, the rate of heat generation due to the exothermal polystyrene polymerization reaction is high, the heat evolved from the reaction is sufficient to maintain the reaction temperature to its set point trajectory. As the reaction proceeds with time, the rate of polymerization reaction decreased and

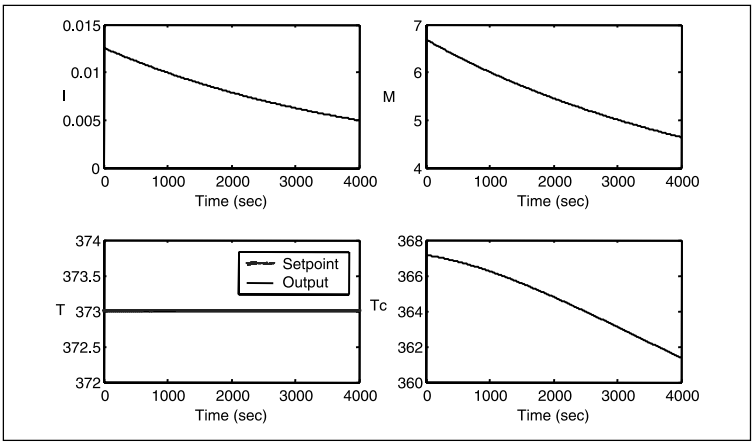

FIGURE 5. Nominal reactor temperature set point.

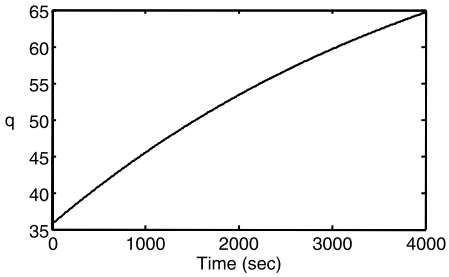

FIGURE 6. Manipulated variable corresponds to nominal temperature set point.

hence the heat generation rate decreases, the MPC control strategy in this case is therefore increases monotonically the input heat to the batch polymerization reactor to keep reactor temperature to its set point profile. At a range of time between 1000 and 4300 seconds, the reactor set point temperature is dropping from 374 K to 371 K; the slight decrease in the reaction temperature set point still required heat to compensate the drop in the heat generation rate (figure 8).

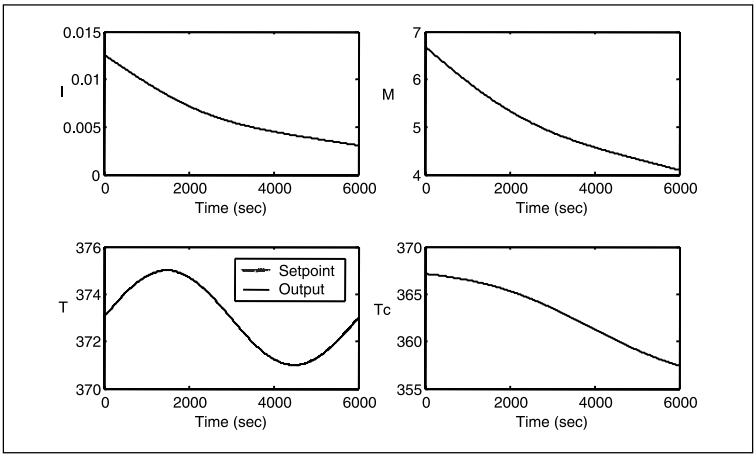

FIGURE 7. Sinusoidal changes in temperature set point.

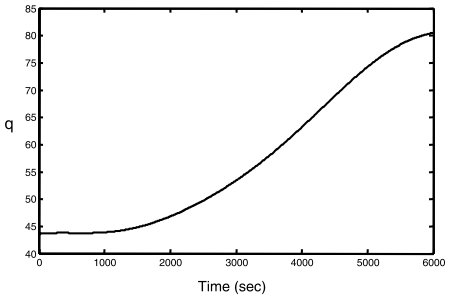

FIGURE 8. manipulated heats transfer the reactor corresponding to sinusoidal change in temperature set point.

3. Tracking the stepwise changes in set point for the reaction temperature

Figure 9 shows the model predictive control response to stepwise change in reactor temperature set point. It can be seen that, during the first 5000 seconds of operation under the MPC controller action, the reactor temperature traced the temperature set point sharply throughout the operation. After 5000 seconds of operation there exists reactor temperature deviation from the set point, this is expected due the depletion of initiator concentration inside the reactor.

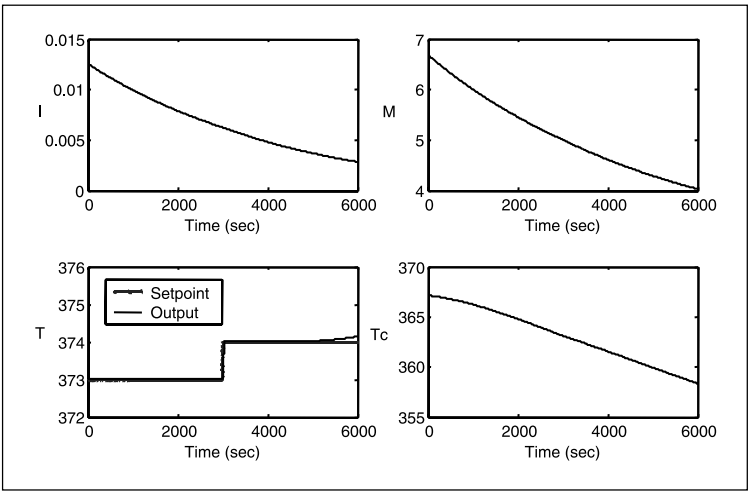

FIGURE 9. Results of tracking the stepwise changes in set point for the reaction temperature by the model predictive control.

Heat added to the reactor as a result of MPC control action increased slightly with increasing time, a sharp increase in heat takes place at the time where a stepwise change in reactor temperature set point is generated. The overshoot took just few second after which the heat regain it original path with slight monotonic increase.

4. Tracking of the optimal temperature trajectory with MPC

In general, the ultimate goal of the polymerization reactor temperature control

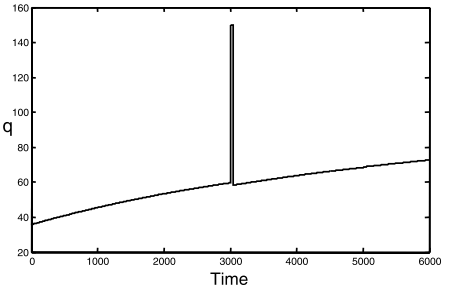

FIGURE 10. Manipulated heat supplied to the batch reactor corresponding to reactor temperature set point change.

is to obtain polymer product having desired properties. Therefore, the batch operation is often carried out for tracking a given temperature trajectory. Figure 11 shows the simulation results for tracking the optimal temperature trajectory which was calculated in an open loop manner. For this the MPC was employed as the master controller

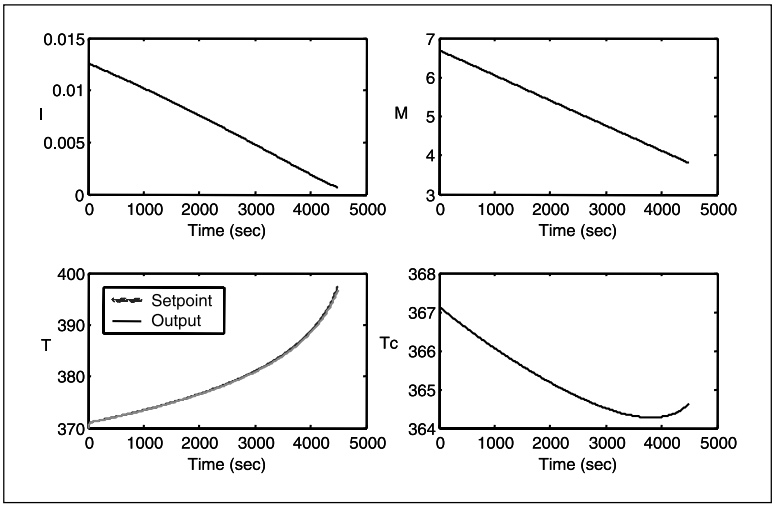

FIGURE 11. Optimum temperature profile of reactor temperature set point.

Figure 11 shows that the reactor temperature traced the optimal trajectory sharply throughout the operation. The initial reactor temperature was close to the set point, a slight deviation from the set point builds up with time.

The difference is minor and is acceptable. Initially, heat supplied to the batch reactor overshoot to 150 w then by time keeps monotonic increase with oscillatory manor (figure 12).

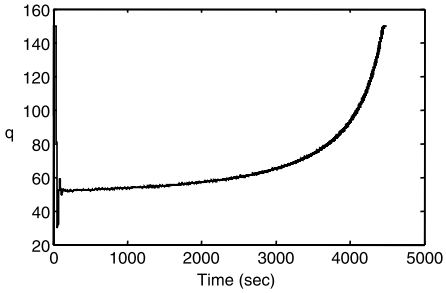

FIGURE 12. Manipulated heat profile corresponding to reactor optimum temperature profile.

CONCLUSION

Model Predictive Control, a non-linear model based controller has several interesting characteristics and suitable for almost any kind of problems. It displays its main strength when applied to problem with a large number of manipulated and controlled variables, constraints imposed on both the manipulated and controlled variables, changing control objectives and/or equipment failure and time delays. In this work, the MPC controller is applied to batch polymerization reactor for polystyrene production. This process is single input single output problem, highly dynamic behavior, and multivariable interaction. The Simulation results have demonstrated that the MPC controller can provide reliable control performance.

6. NOMENCLATURE

$I_{o,}$ I	Initial, Initiator concentration (mol/l)
Q	Heat input (W)
M_o, M	Initial, Monomer concentration (mol/l)
ΔH	Heat reaction (J/mol)
q_o	Zeroth moment
V	Volume (l)
q_2	Second moment
V_c	Jacket volume (l)
A	Area (m^2)
M_c	Coolant flow rate (mol/s)
T	Reactor temperature (K)
T_{ci}	Inlet jacket temperature (K)
T_c	Average jacket temperature (K)
k_d,k_p,k_t	Kinetic constants
T_{co}	Outlet jacket temperature (K)
X_n	Number of average chain length
U	Overall heat transfer coefficient ($W/(m^2K)$
f	Efficiency
C_p	Specific heat capacity of mixture (J/mol.K)
X	Conversion
C_{pc}	Specific heat capacity of coolant (J/mol.K)

Greek letters

ρ	density of the mixture (g/l).
ρ_c	density of the coolant (g/l).

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