Development and Validation of Advanced Nonlinear Predictive Control Algorithms for Trajectory Tracking in Batch Polymerization

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ABSTRACT: In this work, a computationally efficient nonlinear model-based control (NMBC) strategy is developed for a trajectory-tracking problem in an acrylamide polymerization batch reactor. The performance of NMBC is compared with that of nonlinear model predictive control (NMPC). To estimate the reaction states, a nonlinear state estimator, an unscented Kalman filter (UKF), is employed. Both algorithms are implemented experimentally to track a time-varying temperature profile for an acrylamide polymerization reaction in a lab-scale polymerization reactor. It is shown that in the presence of state estimators the NMBC performs significantly better than the NMPC algorithm in real time for the batch reactor control problem.

1. INTRODUCTION

The batch mode of operation is utilized in the production of industrially relevant chemicals when the volume is small and there is significant variety in production. Batch reactors are inherently dynamic in nature, and end-point optimization is typically achieved by following an optimal time-varying trajectory. Be it any batch process, nonlinearities due to reaction kinetics and temperature effects make the control of such processes challenging and also require optimum procedures for efficient operation. The use of model-based control techniques for this class of trajectory-tracking problems has proven to be popular in the literature. The nonlinear model predictive control (NMPC) strategy is a model-based technique where the model states are predicted over a particular number of future time instants and future control variables are obtained by minimizing the error between the set point and the output. The NMPC schemes provide an approximate solution to the optimal control of batch and semibatch polymerization reactors implemented in a receding horizon manner.[8,9] and diminishing horizon manner.[10]

Although various data-driven system identification strategies such as autoregressive with exogenous inputs, i.e., NARX and ARX models,[11,12] Laguerre–Volterra models,[13] neural networks,[14] or Gaussian process models,[15] are used along with NMPC for batch and semibatch processes, using a first-principles model can provide better insight into the dynamics of the system. With online control calculation time being a major issue with NMPC, a control strategy known as nonlinear model-based control (NMBC), which can be considered as a particular case of NMPC with a single prediction and correction step, has proven to provide better performance compared to NMPC in the control of nonlinear processes.[16,17] NMBC involves the calculation of the control signal by solving the model state equations numerically, thereby eliminating the time required for optimization. One common feature of these techniques is the need to have measurements or estimates of the system states. Since reactant concentration measurements are typically not available online in batch chemical reactor systems, it is necessary to employ state observers. The use of an unscented Kalman filter (UKF) has the advantage of incorporating the nonlinear model directly without the need to linearize, and hence the nature of the model is preserved. Successful augmentation of the UKF with NMBC and NMPC controllers can be found in level control and reactor problems.[18–21]

NMBC has only been applied to servo and regulatory control problems in the literature, which involve constant set points and step changes. The contribution of this study is the development of a computationally inexpensive NMBC strategy that can be implemented in a trajectory-tracking problem. The efficacy of this scheme is experimentally validated for an
acrylamide polymerization reaction in a lab-scale batch reactor. The UKF is used to obtain accurate prediction and estimation of states with the available temperature measurements. The tracking performance of UKF-NMBC is compared with that of the nonlinear model predictive controller.

2. THEORETICAL DEVELOPMENT

A nonlinear system, whose states are modeled by ordinary differential equations and outputs are functions of system states, can be represented as follows

\[ \dot{x} = f(x(t), u(t)) \]

\[ y(t) = C_m x(t) \quad (1) \]

where \( x(t) \in \mathbb{R}^n \), \( u(t) \in \mathbb{R}^m \), and \( y(t) \in \mathbb{R}^p \) are the states, inputs, and outputs, respectively. \( C_m \) is the measurement matrix of dimension \( p \times n \). For prediction, the above continuous equations should be discretized. With \( \Delta t \) as the constant step size or sample time, the discrete form of the system equations is given as follows

\[ x(k) = x(k-1) + \int_{(k-1)\Delta t}^{k\Delta t} f(x(t), u(k-1))dt \]

\[ y(k) = C_m x(k) \quad (2) \]

\[ y(k) = C_m x(k) + v(k) \quad (3) \]

2.1. UKF-Based Nonlinear Model-Based Control (UKF-NMBC) for Trajectory Tracking. The nonlinear system affected by random process noises \( w(k) \) and measurements affected by random measurement noises \( v(k) \) are formulated as

\[ x(k) = x(k-1) + \int_{(k-1)\Delta t}^{k\Delta t} f(x(t), u(k-1))dt + w(k) \]

\[ y(k) = C_m x(k) + v(k) \quad (4) \]

The NMBC strategy is formulated as the following five steps.

**Step 1.** The model states are calculated over a single sampling instant. To predict the immeasurable states and to deal with process and sensor noises, the state estimator UKF is used, which works in two steps.18,19,21

UKF prediction: The one-step-ahead predicted state \( \hat{x}(kk+1) \) is obtained using the previous estimate \( \hat{x}(k-1k-1) \) and the model eq 2. Using the predicted error covariance \( P(kk+1) \) and the model equation, the measurement \( \hat{y}(kk+1) \) is predicted.

UKF correction: Using the innovation \( y(kk+1) \), which is the difference between the actual and predicted measurement \( y(k) - \hat{y}(kk+1) \), and the Kalman gain \( K(k) \), which necessarily minimizes the state error covariance using innovation covariance \( P_{yy}(k) \) and innovation cross-covariance \( P_{yx}(k) \), the optimal state estimate \( \hat{x}(kk+1) \) is obtained as \( \hat{x}(kk+1) = \hat{x}(kk+1) + K(k)(y(kk+1) - \hat{y}(kk+1)) \).

**Step 2.** The control signal's value \( u_p(k) \) is calculated by solving the state equation, which involves the control signal. Here, the right-hand side of the state equation is equated to the difference between the one-step-ahead set point and estimated measurement so that the calculated control signal takes the output to the desired set point

\[ C_f(\hat{x}(kk+1), u_p(k))\Delta t = y_p(k+1) - C_p \hat{x}(kk+1) \quad (5) \]

The selection vector \( C_p \) selects the model equation that contains the manipulated variable to be solved above.

**Step 3.** The correction term \( u_p(k) \) for the predicted flow rate is calculated based on the error between the set point and predicted measurement as it is free from noise, multiplied by a proportional gain. The optimal gain can be selected such that it minimizes any of the performance measures19 and can be suitably tuned to get the desired response while implementing in real-time systems

\[ u_p(k) = K_e(k) = K_e(y_p(k) - C_p \hat{x}(kk+1)) \quad (6) \]

**Step 4.** The augmented control input is taken to be the sum of prediction and correction control signals

\[ u_A(k) = u_p(k) + u_p(k) \quad (7) \]

**Step 5.** Further, the control input obtained in Step 4 is subjected to hard constraints, and the controller input \( u(k) \) thus obtained is applied to the system

\[ u(k) = \begin{cases} u_{\text{min}} & \forall \quad u_A(k) \leq u_{\text{min}} \\ u_A(k) & \forall \quad u_{\text{min}} < u_A(k) < u_{\text{max}} \\ u_{\text{max}} & \forall \quad u_A(k) \geq u_{\text{max}} \end{cases} \quad (8) \]

2.2. UKF-Based Nonlinear Model Predictive Control (UKF-NMPC) for Trajectory Tracking. The basic NMPC philosophy involves prediction of plant output over a prediction horizon and calculating the future control actions to minimize a cost function, which accounts for the error between the set-point trajectory and output. A term to minimize control deviation is also included in the cost function so that the manipulated variable does not change rapidly. The optimal estimation of future outputs is achieved by the UKF through innovation-based prediction−correction. The UKF-NMPC algorithm is formulated as follows.

Given a set of future set points, \( y_p(k+jk), \forall j = 1...N_p \), with \( N_p \) being the prediction horizon. The future control actions \( u(k), u(k+1k), u(k+1) \) \( \ldots u(k+N_k-1k) \) with the control horizon \( N_k \) are calculated, which minimizes the objective function

\[ J = \min_{u(kk)} \sum_{j=1}^{N_p} W_j(E^2(k+jk)) \]

\[ + \sum_{j=0}^{N_k-1} W_k(\Delta u^2(k+jk)) \quad (9) \]

where

\[ E(k+jk) = y_p(k+jk) - \hat{y}(k+jk), \forall j = 1 \ldots N_p \]

\[ \Delta u(k+jk) = u(k+jk) - u(k+j-1k), \forall j = 0 \ldots N_k - 1 \quad (10) \]

subject to constraints

\[ u_{\text{min}} \leq u(k+jk) \leq u_{\text{max}}, \forall j = 0 \ldots N_k - 1 \]

\[ \Delta u(k+N_kk) = \Delta u(k+N_k-1k) \]

\[ = \ldots \Delta u(k+N_k-1k) = 0 \quad (11) \]
The first control action \( u(\text{clk}) \) obtained after minimization is implemented in the system. The remaining set of control actions is subjected to reoptimization, implementing a receding horizon strategy. The weights on output error \( W_e \) and control deviation \( W_u \) take care of tracking and smooth control variations.

The calculation of a future set of outputs \( \hat{y}_m \) using the UKF involves the following steps.

**Step 1.** Sigma points \( \chi(kl) \) are generated by starting with the current estimate (mean) \( \hat{x}_m(\text{clk}) \), state error covariance \( P(\text{clk}) \), and model. Here, the first and second moments of the state, i.e., mean and variance, are used to transform the distribution through the model; hence, sigma points approximate the distribution to be Gaussian

\[
\chi(\text{clk}, 0) = \hat{x}_m(\text{clk})
\]

\[
\chi(\text{clk}, l) = \hat{x}_m(\text{clk}) + (\sqrt{(n + \lambda)P(\text{clk})})_l, \quad l = 1, 2, ..., n \]

\[
\chi(\text{clk}, l) = \hat{x}_m(\text{clk}) - (\sqrt{(n + \lambda)P(\text{clk})})_{-l, l} = n + 1, n + 2, ..., 2n
\]

(12)

Here, \( \lambda \) decides the arrangement of sigma points, i.e., the mean, and is given by \( \lambda = \alpha^2 (n + \kappa) - \kappa; \) the closeness of sigma points to the mean is directly proportional to the value of \( \alpha \) and square root of \( \kappa \), and \( n \) is the dimension of the state vector.

**Step 2.** The unscented transformation is performed using the nonlinear model, and a future set of sigma points over the prediction horizon \( N_p \) is obtained, which results in a multistep-ahead prediction

\[
\chi(k + j + 1\text{lk}, l) = \chi(k + j, l) + f(\chi(k + j, l), u(k + j|l))\Delta t,
\]

\[\forall l = 0, 1, ..., 2n \text{ and } j = 0, 1, ..., N_p - 1\]

(13)

The transformed sigma points are weighted to correct the predicted mean and error covariance, since inclusion of the mean in sigma points affects the variance of the transformed distribution. The corresponding weights of each \( 2n + 1 \) sigma point are given as follows

\[
W^m(0) = \frac{\lambda}{n + \lambda}
\]

\[
W^c(0) = \frac{\lambda}{n + \lambda} + (1 - \alpha^2 + \beta)
\]

\[
W^c(j) = W^m(j) = \frac{1}{2(n + \lambda)}, \quad j = 1, 2, ..., 2n
\]

(14)

The value of \( \beta \) incorporates the knowledge of noise distribution and is set equal to zero when information is not available.

**Step 3.** The predicted mean is calculated as the weighted sum of the sigma points

\[
\hat{x}_m(k + j + 1\text{lk}) = \sum_{j=0}^{2n} W^m(j)\chi(k + j + 1\text{lk}, l), \quad \forall j
\]

\[= 0, 1 ... N_p - 1\]

(15)

The so-obtained mean is corrected using the Kalman gain \( K \) and innovation \( \gamma \), which reduces the estimation error

\[
\hat{x}_m(k + j + 1\text{lk}) = \hat{x}_m(k + j|l) + K(k)\gamma(k|l-1), \quad j
\]

\[= 0, 1 ... N_p - 1\]

(16)

The Kalman gain, which is obtained such that it minimizes the trace of the error covariance matrix, thus accounts for optimality of the Kalman filter. The Kalman gain is calculated as

\[
K(k) = P_{ee}(k)[P_{ee}(k)]^{-1}
\]

(17)

The innovation covariance \( P_{ee} \) and cross-covariance \( P_{ev} \) are calculated as follows

\[
P_{ee}(k) = \sum_{j=0}^{2n} \{W^e(i)[C_m\chi(\text{clk} - 1, i) - \hat{y}_m(\text{clk} - 1)]\times
\]

\[C_{me}^{*}(\text{clk} - 1, i) - \hat{y}_m(\text{clk} - 1)]^T \} + R
\]

(18)

\[
P_{ev}(k) = \sum_{j=0}^{2n} \{W^e(i)[C_m\chi(\text{clk} - 1, i) - \hat{x}_m(\text{clk} - 1)] \times
\]

\[C_{Mk}^{*}(\text{clk} - 1, i) - \hat{y}_m(\text{clk} - 1)]^T \}

(19)

where \( R \) is the measurement noise covariance. The innovation is the difference between the actual measurement \( y_m(k) \) and predicted measurement \( \hat{y}_m(k|l - 1) \)

\[
\gamma(k|l - 1) = y_m(k) - \hat{y}_m(k|l - 1)
\]

(20)

It should be noted that calculations 17–20 are performed in advance while estimating \( \hat{x}_m(\text{clk}) \). The state error covariance is updated using the state innovation and process noise covariance \( Q \)

\[
P(k + j + 1\text{lk}) = \sum_{j=0}^{2n} W^e(i)\chi(k + j + 1\text{lk}, l)
\]

\[= \hat{x}_m(k + j + 1\text{lk}))
\]

\[
\chi(k + j + 1\text{lk}, l) = \chi(k + j, l) - \hat{x}_m(k + j + 1\text{lk}))\}
\]

\[+ Q, \forall j = 0, 1 ... N_p - 1\]

(21)

**Step 4.** To get the exact distribution of sigma points, they are redrawn from the predicted mean and covariance. This step can be dropped to save computational time, but inclusion of redrawn sigma points results in a more accurate state estimation

\[
\chi^{*}(k + j|l, 0) = \hat{x}_m(k + j|l), \quad \forall j = 0, 1 ... N_p - 1
\]

\[
\chi^*(k + j|l, l) = \hat{x}_m(k + j|l) + (\sqrt{(n + \lambda)P(k + j|l))},
\]

\[\forall l = 1, ..., n \text{ and } j = 0, 1 ... N_p - 1\]

\[
\chi^*(k + j|l, l) = \hat{x}_m(k + j + 1\text{lk}) - (\sqrt{(n + \lambda)P(k + j|l))})_{-l, l}
\]

\[\forall l = n + 1, ..., 2n \text{ and } j = 0, 1 ... N_p - 1\]

(22)
The predicted output is obtained from the redrawn sigma points and output equation as follows

$$
\hat{y}_m(k + jlk) = \sum_{l=0}^{2N_p} W^m(l) C_{w,dl}^n(k + jlk, l), \forall j
$$

$$
= 0, 1, \ldots, N_p - 1
$$

(23)

Step 5. Using the innovation at the current instant $\gamma(klk) = y_m(k) - C_{w,dl}^n(klk)$ to filter out the effect of noises, the predicted measurements are obtained as follows

$$
\hat{y}_m(k + j + 1lk) = \hat{y}_m(k + j + 1lk) + \gamma(klk), \forall j
$$

$$
= 0, 1, \ldots, N_p - 1
$$

(24)

The so-obtained predicted set of measurements is used in the objective function to obtain the optimal control sequence, and the first control element is employed in the system with the rest of them subjected to reoptimization.

3. APPLICATION TO BATCH POLYMERIZATION

3.1. System Dynamics of the Batch Reactor. The batch reactor’s system dynamics involves the reaction kinetics, reactor, and jacket energy balance equations. This study makes use of an acrylamide polymerization reaction, with initiator ammonium persulfate concentration $[I]$ and monomer acrylamide concentration $[M]$ modeled as follows

$$
\frac{d[I]}{dt} = -A_d[I]e^{(-E_d/R(T_k+273.15))}
$$

(25)

$$
\frac{d[M]}{dt} = -A_p[I]^\theta [M]^{\theta }e^{(-E_p/R(T_k+273.15))}
$$

(26)

The reactor temperature $T_r$ and jacket temperature $T_j$ dynamics are given by

$$
m_c \epsilon_p \frac{dT_r}{dt} = Q_R - UA(T_r - T_j) + Q_h + Q_s - Q_{loss}
$$

(27)

$$
m_c \epsilon_{pf} \frac{dT_j}{dt} = UA(T_r - T_j) - F_c \epsilon_{pc}(T_j - T_c)
$$

(28)

where

$$
Q_R = \frac{d[M]}{dt} V \Delta H_p
$$

(29)

$$
Q_s = \rho \rho m^3 d^5
$$

(30)

$$
Q_{loss} = \alpha(T_j - T_{amb})^\beta
$$

(31)

$$
m_c \epsilon_{pi} = \sum_{i=1}^{6} m_c \epsilon_{pi}
$$

(32)

$$
m_c \epsilon_{pj} = \sum_{i=7}^{8} m_c \epsilon_{pi}
$$

(33)

The overall heat transfer coefficient $U$ is calculated based on the time constant of the batch reactor, and the heat loss coefficients $\alpha$ and $\beta$ are estimated in a least-squares sense.24

3.2. UKF-NMBC for the Batch Reactor. The calculation of manipulated variable $F_c$ through UKF-NMBC with system-specific equations and procedures is reported below. The system ODEs are represented in discrete form as follows

$$
\begin{bmatrix}
[I] \\
[M] \\
T_r \\
T_j
\end{bmatrix}_{k} =
\begin{bmatrix}
[I] \\
[M] \\
T_r \\
T_j
\end{bmatrix}_{k-1} - A_d[I]e^{(-E_d/R(T_k+273.15))}
$$

$$
+ A_p[I]^\theta [M]^{\theta }e^{(-E_p/R(T_k+273.15))} + [Q_R - UA(T_r - T_j) + Q_h + Q_s - Q_{loss}] / m_c \epsilon_{pc}
\]

$$
\left[UA(T_r - T_j) - F_c \epsilon_{pc}(T_j - T_c)\right] / m_c \epsilon_{pf}
$$

\Delta t

(34)

The measurements from the system are obtained from states at the time instant $k$ as

$$
\begin{bmatrix}
T_r \\
T_j
\end{bmatrix}_{k} =
\begin{bmatrix}
0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0
\end{bmatrix}
\begin{bmatrix}
[I] \\
[M] \\
T_r \\
T_j
\end{bmatrix}_{k}
$$

(35)

The states and measurements are affected by the random process and measurement noises. This creates a need for filters to provide noise-free estimates of the states. The UKF uses the measurements available at the current instant to estimate the optimal states. The estimated states are represented as

$$
\begin{bmatrix}
[I] \\
[M] \\
T_r \\
T_j
\end{bmatrix}_{\hat{k}}
$$

(36)

For the batch reactor model, the manipulated variable is the coolant flow rate $F_c$, which appears in the jacket temperature dynamics. Therefore, the set point required for the jacket is predetermined using the initiator, monomer, and reactor model equations by propagating the reactor set point. Since tracking of the jacket set point implies tracking that of the reactor, this requires the jacket temperature to be equal to the jacket set point $T_{j,sp}$ at every instant

$$
T_{j,sp}(k + 1) = T_j(k)
$$

$$
\left[UA(T_r(k) - T_j(k)) - F_c(k) \epsilon_{pc}(T_j(k) - T_c)\right] / m_c \epsilon_{pf}
\]

\Delta t

(37)

Using the UKF-estimated values in eq 37 and rearranging them, we get the following

$$
\left[UA(T_r(k) - T_j(k)) - F_c(k) \epsilon_{pc}(T_j(k) - T_c)\right] / m_c \epsilon_{pf}
\]

$$
\Delta t

(38)

Solving eq 38 for $F_c(k)$, this flow rate takes the jacket temperature to the required set point. The correction term that accounts for unmeasured disturbances and modeling error can be taken as the proportional gain multiplied by the difference between the jacket set point and measured temperature.
A positive error implies that flow should be decreased and vice versa. Therefore, the corrected flow rate here is subtracted from the predicted flow rate. The modified flow rate is given by

$$
F_{c}(k) = \hat{F}(k) - \bar{F}(k)
$$

Furthermore, the hard constraints on the flow rate are applied by projecting the values outside the limits to its boundary.
Here, the maximum and minimum flow rates are $F_{\text{max}} = 0.75 \text{ lpm}$ and $F_{\text{min}} = 0 \text{ lpm}$, respectively. The specific batch polymerization reactor equations developed here are used with the general procedure outlined in Section 2 to implement UKF-NMBC and UKF-NMPC in the next section.

4. EXPERIMENTAL APPLICATION

4.1. Development of the Experimental Facility. The experimental studies are carried out at a lab-scale batch reactor facility in the Department of Instrumentation and Control Engineering Lab-2, MIT Manipal. The system’s major components are a reactor vessel, heater, cooling coil, stirrer, and flow control station as shown in Figure 1. The reactor vessel and serpentine cooling coil are made of 316 SS material and have a maximum capacity of 1 L and 18 mL, respectively, as shown in Figure 2. A 1 kW ceramic band heater of 1500 W 230 V is used to heat the reaction mixture. There is no physical contact between the heater and reactor vessel to avoid rust formation, and process heating is via radiation. The heater supply is maintained constant at 50%, and the coolant flow rate is used as the manipulated variable. The reactor can handle a pressure of up to 30 bar.

A uniform heating of reactants is achieved by a stirrer coupled with a motor with operating speed set to 200 rpm throughout this study. A reverse-acting flow control valve is used to manipulate the coolant flow rate (0–0.75 lpm) to maintain the desired temperature. Figure 3 presents the schematic of the entire setup comprising a PC running the control algorithm, flow station, and pilot plant.

The interface between the computer and the pilot plant is done through an ACE 2002 data acquisition (DAQ) card, which interacts with the PC through Wi-Fi communication. It works on a 24 V DC supply, and the input–output signals are provided in the range 4–20 mA.

4.2. Reactor Feed and Set Point. The reaction mixture for the acrylamide polymerization reaction is selected to be 500 mL of 10% monomer (acrylamide) and 5 mL of 0.009 mol/L initiator (ammonium persulfate) solution. The temperature profile chosen can have a profound impact on the conversion of the monomer as well as the number-average molecular weight of the final product. In this work, a temperature profile that gives 50% conversion for a batch time of 1 h is used as the set point. This profile ensures that the final product is not close to the gel point and the viscosity of the final product is within the desired product specifications. Initially, the monomer solution is heated, and then the initiator is introduced into the reactor to start the reaction.

4.3. Algorithm and Model Parameters for UKF-NMBC and UKF-NMPC. The plant model with four states given by eqs 25–28 is employed for real-time studies. The estimations of the initiator and monomer concentrations are given by the UKF. The initial estimates of states and algorithm parameters are given in Table 1 and the model parameters are given in Table 2.

A sample time of 1 s for updating the control action is used for UKF-NMBC, and the MATLAB numerical solver `vpasolve` is used to get the predicted control signal $u_k$. To account for the computation time involved in UKF-NMPC, a sample time of 2 s is used, and the MATLAB optimization routine `fmincon` is used to get the predicted control signal $u_k$.

### Table 1. Algorithm and UKF Parameter Values for Experimental Studies

| parameter                  | value                          |
|----------------------------|-------------------------------|
| initial state estimate, $\hat{x}(0)$ | $[4.5 \times 10^{-3}, 0.7034, 55, 36.8]^T$ |
| NMBC gain, $K_c$            | 2                             |
| NMPC prediction and control horizon weights $W_k$ and $W_u$ | $5$ and $0.5$, respectively |
| $P(0)$                     | $\text{diag}(0.000005^2, 0.0005^2, 0.5^2, 0.5^2)$ |
| $Q_k$                      | $\text{diag}(0.000005^2, 0.0005^2, 0.01^2, 0.01^2)$ |
| $R_k$                      | $\text{diag}(0.1^2, 0.1^2)$   |
| $\xi_n$                    | $[0 \ 0 \ 0 \ 1]$             |
| UKF tuning parameters      | $\alpha = 0.5, \beta = 0, \kappa = 0.5$ |

### Table 2. Model Parameter Values Used for Experimental Studies

| parameter | value                          | parameter | value                          |
|-----------|--------------------------------|-----------|--------------------------------|
| $A_b$     | $4.4 \times 10^{16} \text{ s}^{-1}$ | $m_1$     | $450 \text{ g}$               |
| $A_p$     | $2.833 \times 10^9 \text{ L}^{0.75} \text{ mol}^{-0.75} \text{ s}^{-1}$ | $m_2$ (initial) | $4.5 \times 10^{-3} \text{ mol}$ |
| $E_b$     | $140.06 \times 10^3 \text{ J}$ | $m_3$ (initial) | $0.7034 \text{ mol}$           |
| $E_p$     | $7.0711 \times 10^4$       | $m_4$ (initial) | $0 \text{ mol}$               |
| $R$       | $8.3145 \text{ J mol}^{-1} \text{ K}^{-1}$ | $m_5$     | $220 \text{ g}$               |
| $e$       | $0.5$                        | $m_6$     | $7200 \text{ g}$              |
| $\theta$  | $1.25$                       | $m_7$     | $18 \text{ g}$                |
| $V$       | $0.5 \text{ L}$             | $m_8$     | $240 \text{ g}$               |
| $\Delta H_p$ | $-82.2 \times 10^3 \text{ J} \text{ mol}^{-1}$ | $\xi_1$  | $4.184 \text{ J} \text{ g}^{-1} \text{ C}^{-1}$ |
| $UA$      | $27.0283 \text{ W} \text{ C}^{-1}$ | $\xi_2$  | $187 \text{ J} \text{ mol}^{-1} \text{ C}^{-1}$ |
| $Q_b$     | $650 \text{ W}$            | $\xi_3$  | $110.58 \text{ J} \text{ mol}^{-1} \text{ C}^{-1}$ |
| $\rho_s$  | $10.72305$                  | $\xi_4$  | $84.95 \text{ J} \text{ mol}^{-1} \text{ C}^{-1}$ |
| $\rho$    | $1000.05 \text{ kg m}^{-3}$ | $\xi_5$  | $0.49 \text{ J} \text{ g}^{-1} \text{ C}^{-1}$ |
| $n$       | $200 \text{ rpm} = 3.33 \text{ rps}$ | $\xi_6$  | $0.49 J \text{ g}^{-1} \text{ C}^{-1}$ |
| $d$       | $0.05 \text{ m}$           | $\xi_7$  | $4.184 \text{ J} \text{ g}^{-1} \text{ C}^{-1}$ |
| $\alpha$  | $1.0003 \text{ W} \text{ C}^{-2}$ | $\xi_8$  | $0.49 \text{ J} \text{ g}^{-1} \text{ C}^{-1}$ |
| $\theta$  | $27 \text{ C}$              | $T_{\text{amb}}$ | $27 \text{ C}$               |
with a sequential quadratic programming (SQP) solver is used for optimization. The initial reactor and cooling coil temperatures are taken to be 55 and 36.8 °C, respectively; the same values are taken to be the initial estimate for the UKF. The manipulated variable, the coolant flow rate, is constrained between 0 and 0.75 lpm, and the coolant temperature is assumed to be equal to ambient temperature.

5. RESULTS AND DISCUSSION

From the experimental results shown in Figure 4, it can be clearly noted that UKF-NMBC provides satisfactory tracking and the output is close to the set point throughout the batch time. Overshoot and large offset are observed for the case of UKF-NMPC. Although the manipulated variable, i.e., the coolant flow rate varies rapidly for UKF-NMBC, it is comparable to the smooth varying UKF-NMPC flow rate. The sum of squared errors (SSE) given in Table 3 confirms the tracking efficiency of UKF-NMBC.

The conversion of the monomer to polymer given in Figure 5 is higher for UKF-NMPC as we can infer from Figure 4 that its temperature profile is above the set point for most of the time. This higher temperature leads to the formation of an off-spec product that is not of the desired viscosity and number-average molecular weight. On the other hand, the monomer conversion for UKF-NMBC is close to the expected conversion, which leads to the formation of a final product of the desired specifications of viscosity and number-average molecular weight.

6. CONCLUSIONS

In this work, a computationally inexpensive NMBC for a trajectory-tracking problem is presented with experimental validation in comparison with NMPC. The tracking capability of the controller along with the UKF for state estimation is tested experimentally for a dynamic set-point tracking problem for an acrylamide polymerization reaction in a lab-scale batch reactor. It is shown that UKF-NMBC provides better tracking compared to UKF-NMPC, which in turn results in the formation of a polymer product of the desired end-point properties in a batch reactor.

Table 3. Comparison of SSE Values for UKF-NMBC and UKF-NMPC

| algorithm   | SSE        |
|-------------|------------|
| UKF-NMBC    | 2.2989 × 10^3 |
| UKF-NMPC    | 8.8775 × 10^3 |

Figure 4. Closed-loop control of the pilot plant batch reactor. A comparison of UKF-NMBC with UKF-NMPC.

Figure 5. Estimated monomer conversion. A comparison of UKF-NMBC with UKF-NMPC.
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Notes
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NOMENCLATURE

- $I$: initiator concentration
- $M$: monomer concentration
- $\alpha$, $\beta$: heat loss coefficients
- $\Delta H_p$: heat of polymerization
- $\varepsilon$, $\theta$: reaction constants
- $A$: area of heat transfer
- $c_p$: specific heat of the solvent
- $c_{p1}$, $c_{p2}$, $c_{p3}$: specific heat of the initiator
- $c_{p4}$, $c_{p5}$, $c_{p6}$: specific heat of the polymer
- $c_{p7}$, $c_{p8}$, $c_{pc}$: specific heat of the coolant fluid
- $c_{pb}$, $c_{pc}$: specific heat of the cooling coil
- $d$: diameter of the stirrer blades
- $E_d$: dissociation enthalpy
- $P_i$: polymerization enthalpy
- $F_c$: coolant flow rate
- $m_1$: mass of the solvent (water)
- $m_2$: number of moles of the initiator
- $m_3$: number of moles of the monomer
- $m_4$: number of moles of the polymer
- $m_f$: mass of the stirrer
- $m_r$: mass of the reactor vessel
- $m_c$: mass of the coolant fluid
- $m_l$: mass of the cooling coil
- $n$: rotational speed of the stirrer
- $P_0$: power number
- $Q_h$: heat added to the reactor
- $Q_f$: heat due to the reaction
- $T_c$: coolant temperature
- $T_j$: jacket temperature
- $T_u$: universal gas constant
- $T_{amb}$: ambient temperature
- $U$: overall heat transfer coefficient
- $V$: volume of the reaction mixture
- $A_d$: dissociation constant
- $A_p$: polymerization constant
- $\rho$: density of the reaction mixture

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