International Academic Institute for Science and Technology

International Academic Journal of Science and Engineering
Vol. 12, No. 4, 2025, pp. 186-196.

ISSN 2454-3896

International Academic Journal of Science and Engineering

www.iaiest.com

Computational Analysis of Reactor Temperature Control of Batch Polymerization Process

M. Valluvan [a], Dr.G. Sakthivel [b]

[a] *Research Scholar, Department of Electronics and Instrumentation Engineering, Annamalai University, Chidambaram, Tamil Nadu, India. E-mail: varunvalluvan@gmail.com, Orcid: https://orcid.org/0009-0002-1302-1858*

[b] *Professor, Department of Electronics and Instrumentation Engineering, Annamalai University, Chidambaram, Tamil Nadu, India. E-mail: gsauei@gmail.com, Orcid: https://orcid.org/0000-0002-4868-5614*

Abstract

Batch reactor is non-linear process plays major role in many chemical industries. Modeling and controlling of its parameters are very ambitious job. Because generalized modeling is not suitable all kinds of batch process, apart from general parameters, each batch has its own governing parameters. The common parameter plays major role in batch reactor are reactor temperature and coolant Jacket temperature. controlling reactor temperature helps in achieving desired final product. In this work polymerization batch reactor is taken for computational analysis and Autoregressive exogenous model is identified for reactor temperature profile by lease mean square estimation technique. The developed model is used as a reference model for nonlinear model-based controller, whose control parameters are estimated by Unscented Kalman Filter (UKF) and Extended Kalman Filter (EKF). Additionally, conventional cascade control is developed by traditional method and Unscented Kalman Filter (UKF), Extended Kalman Filter (EKF) are deployed to identify PID controller gain values. The results of all the developed control strategies are analyzed by performance indices. the best fit control strategies are highlighted and recommended for future analysis.

Keywords: Autoregressive Exogenous ARX, Extended Kalman Filter-Nonlinear Model-Based Controller EKF Nmbc, Initiator Ammonium Persulphate Concentration I, Jacket Temperature T_j, Least Mean Square Lms, Monomer Concentration M, Nonlinear Autoregressive Exogenous NARX, Output Y, Reactor Temperature T_r, Unscented Kalman Filter-Nonlinear Model-Based Controller UKF NMBC.

Introduction

Temperature control of batch reactor is a most important task in industry. Because ambient temperature profile of batch reactor facilitates successful product formation. Batch process is a cascade control system. though batch process is highly nonlinear, the process should be linearized at basic constraints to the implementation of conventional PID controllers in primary and secondary control loops of cascade control. In many cases the system cannot be linearized because of nonlinearity profiles of the system, in those cases instead of conventional PID model-based control schemes give us better results. In some cases, Nonlinear Model Based control schemes too shows some difficulties in controlling, for that some optimization techniques are helpful for us to identifying controller parameters. In this work unscented Kalman filter and extended Kalman filter are employed for estimating Nonlinear model-based controller parameters, which will help us to implement best control strategy to the process.

This work addresses, the autoregressive exogenous ARX, NARX model identification by least mean square estimation algorithm. The best fit reactor temperature model of ARX and NARX for batch rector are proposed in this research work and compared with the previously proposed models (Yadav et al., 2021). The best fit model is considered as a

DOI: 10.71086/IAJSE/V12I4/IAJSE1288
Received: 02 October 2025/Revised: 08 November 2025/Accepted: 08 December 2025/Published: 30 December 2025

reference model for Unscented Kalman filter based non-linear model-based controller and Extended Kalman filter based nonlinear model-based controller. The NARX model is compatible for more complex systems (Mahadi et al., 2022), based on this suggestion, it also considered for model validation of the reactor temperature of batch rector (Subramaniam, 2025).

Batch rector is cascade control system, in which reactor temperature is indirectly govern by the coolant jacket temperature. So conventional PID control is implemented for temperature profile control and its results are analyzed (Fathima Sapna, 2021; Bae et al., 2020; Van De Geer, 2005). Unscented Kalman Filter, Extended Kalman Filter algorithms are deployed for the identification of the PID controller gain values and the both the responses are compared for identifying best temperature profile tracking. Unscented Kalman filter based Nonlinear model-based controller (Yadav et al., 2021), Extended Kalman Filter based Nonlinear model-based controller are developed for the temperature profile tracking of batch process

In this work, simulation-based analysis is held for identifying best control strategies for batch process reactor temperature control. So, the differential equations of the batch polymerization process (Yadav et al., 2021) are considered as plant. The data are generated by solving plant differential equations. The collected plant data is subjected to create autoregressive exogenous models (Mahadi et al., 2022; Arasu et al., 2016; Balakrishnan et al., 2023). The best fit reference model is employed in Unscented Kalman Filter based Nonlinear Model based Control (Yadav et al., 2021) and Extended Kalman Filter based Nonlinear Model based control. Extended Kalman Filter is chosen, because in many cases it is employed for nonlinear parameter estimation (Prakash et al., 2010; Chitralekha et al., 2009; Prakash et al., 2010) and gives better result alongside Unscented Kalman Filter based estimation. But in literature Unscented Kalman filter based nonlinear model-based controller alone was developed (Yadav et al., 2021), this is the reason behind in the selection of Extended Kalman Filter for the analysis.

Batch reactor characteristics and its working principles are studied (Mehrani et al., 2022; Rahrooh & Shepard, 2009) for the better understanding of the process. Data scaling is important in data driven model development, so the complete methodology involved are studied (Kumar et al., 2011). Nonlinear model-based controller for conical tank process (Kumar et al., 2011) gives a detail overview of NMBC development and implementation. State estimation based Unscented Kalman filter Nonlinear model-based control (Yadav et al., 2021; Prakash et al., 2010), Nonlinear model-based controller for batch reactor (Rahrooh & Shepard, 2009) elaborates mathematical steps involved in the UKF-NMBC, EKF-NMBC development. The input, output, error orders are chosen precisely to frame the structure of Autoregressive exogenous models (Rahrooh & Shepard, 2009; Mahadi et al., 2022). Least square estimation algorithm is used for the parameter estimation of the reference model (Arasu et al., 2016). Unscented Kalman Filter and Extended Kalman Filter were implemented for three phase machine model parameter estimation (Prakash et al., 2010) gives detail information of mathematical implementation Unscented Kalman Filter and Extended Kalman Filer, based on this PID parameter estimation is done in this work. Additionally, constrained state estimation principles (Chitralekha et al., 2009; Prakash et al., 2010; Serrano & Rossell, 2019) is studied for the support for estimation algorithm development. All the developed control strategies are compared and analyzed based on the performance index. The performance Index chosen in this work is control effort, the energy required for final control element to make faster response based on control action is called as control effort, because higher the control effort value faster the control action.

Batch Polymerization Reactor

The complete configuration of the batch polymerization reactor system is illustrated in fig. 1. The reactor is integrated with a computational interface through a data acquisition module, enabling real-time monitoring and control of process variables. The system is designed to facilitate controlled polymerization reactions under regulated thermal and mixing conditions. The reactor setup incorporates a heat exchange mechanism that ensures efficient thermal regulation during the reaction process, which is critical for maintaining reaction stability and product quality. An external heating arrangement is employed to initiate and sustain the required reaction temperature, while a cooling system is integrated to remove excess heat generated due to exothermic reactions. To achieve uniform composition and temperature distribution within the reactor, a mechanical agitation system is utilized, enhancing mass and heat transfer characteristics. The control architecture includes automated valve systems and instrumentation that allow precise manipulation of process parameters such as temperature, pressure, and flow conditions. Overall, the reactor system is structured to support dynamic operation, providing flexibility for experimental studies, process optimization, and advanced control strategy implementation in polymerization processes.

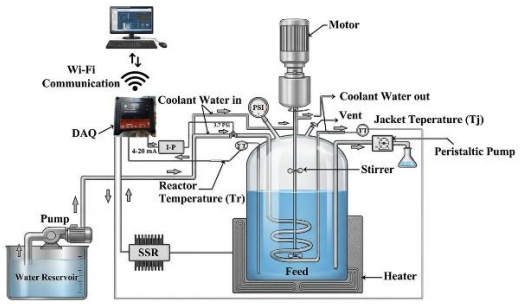

Fig. 1: Schematic of Batch Polymerization Reactor

Mass Balance

$$\frac{d[I]}{dt} = -A_d[I]e^{(-E_d/R(T_r+273.15)} \quad (1)$$

$$\frac{d[M]}{dt} = -A_P[I][M]e^{(-E_P/R(T_r+273.15)} \quad (2)$$

$$m_r c_{pr} \frac{dT_r}{dt} = Q_R - UA(T_r - T_j) + Q_h + Q_s - Q_{loss} \quad (3)$$

$$m_r c_{pj} \frac{dT_j}{dt} = UA(T_r - T_j) - F_c C_{pc}(T_j - T_c) \quad (4)$$

$$Q_R = \frac{d[M]}{dt} V \Delta H_p \quad (5)$$

$$Q_s = P_0\, \rho n^3 d^5 \quad (6)$$

$$Q_s = \propto (T_r - T_{amb})^{\beta} \quad (7)$$

$$m_r c_{pr} = \sum_{i=1}^{6} m_r c_{pr} \quad (8)$$

$$m_j c_{pj} = \sum_{i=7}^{6} m_i c_{pi} \quad (9)$$

The open loop test is conducted by the following considerations[1,2], the initial values of reactor and jacket temperature are taken as 55°Cand 36.8 °C, the refrigerant flow is maintained as 0 and 0.75 Lpm which is equivalent to 0.1 Kg/s, assume coolant temperature and ambient temperature are equal (1). The reaction mixture values are preferred as 500mL of 10% monomer and 5mL of 0.009 mol/L[1] and consider [$Q_{h\ Fc}$] = [60 70] to reach baseline equilibrium and then by input shift of [60 50].[2] Open loop and closed loop analysis are done in MATLAB simulation environment. Temperature profile Y_{water} is 60-20$^{e\text{-}0.0002*(10\hat{}0.1)\ t.}$

System Identification and Parameter Estimation

Modelling of ARX, NARX for reactor temperature has been carried out in this work. General structure of ARX, NARX (2), given by the Equation 10 and Equation 11. the input, output and error orders are n_u=1, n_y=2 and n_e=2.

$$y(t)_{ARX} = \sum_{i=0}^{n_u} a(i)u(t-i) + \sum_{j=1}^{n_y} b(j)y(t-j) + e(t) \quad (10)$$

ARX is linear model in system identification method. This model considers relationship between all variables involved in the process is linear, including error. In general, it is straightforward model. NARX model is an extended version ARX model, which have nonlinear function for mapping past inputs and outputs to current outputs, it includes current prediction error, which simplifies the training of the model.

$$y(t)_{NARX} = \sum_{i=0}^{n_u} a(i)(u(t-i) + \sum_{j=1}^{n_y} b(j)y(t-j) + \sum_{i=0}^{n_u}\sum_{j=1}^{n_u} A(i,j)u(t-i)u(t-j) + \sum_{i=1}^{n_y}\sum_{j=i}^{n_y} B(i,j)y(t-i)y(t-j) + \sum_{j=1}^{n_y} c(i,j)u(t-i)y(t-j) + e(t) \quad (11)$$

Least Mean Square Estimation

Least mean square is estimation technique, which is used to estimate the model parameters (1). The basic structure of lms is given in Equation 12.

$$y = Ax + z \quad (12)$$

Where, vector x∈ $R^{n\times 1}$ is going to be estimated and vector y∈ $R^{m\times 1}$is observation vector, A∈ $R^{m\times n}$ is a data matrix

and z∈ $R^{m\times1}$ is a gaussian noise vector. The lms algorithm solves the unconstrained minimization problem,

$$min_{\hat{x}}\|y - A\hat{x}\|\frac{2}{2} \qquad (13)$$

lms is adaptive filter that works on gradient descent approach to minimize the mean square error based on the latest data it receives. By minimizing the residual error, the x matrix is going to be estimated. x vector is identified by the following Equation 14.

$$x_{ls}=(A^TA)^{-1}A^Ty \qquad (14)$$

This is simple straightforward method of estimation algorithm. By having input and output data, it can estimate the model parameters by minimizing the mean error. NARX model fit best to the reactor temperature profile, when compared with ARX model (1). Based on the literature NARX model is chosen as reference model for Nonlinear model-based control scheme.

Cascade Control

Cascade control scheme block diagram is shown in fig. 2, it comprises of two loops, primary and secondary loop (10), (11). Primary loop comprises of reactor control and secondary loop comprises of coolant jacket temperature control (9), (10).

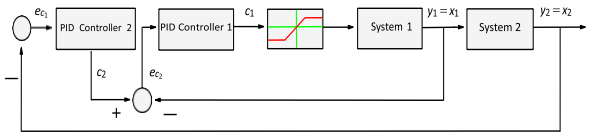

Fig. 2: Schematic of Cascade Control Scheme

Primary PID is tuned by Ziegler Nichols 1 tuning technic, secondary PI controller is tuned by Ziegler Nichols 2 tuning technic. The tuned controller parameters are showed in table 1.

Table 1: PID Controllers Gain Value

Controller		K_p	K_i	K_d
PID	Primary loop	0.08	0.00004	160
	Main loop	1.2	0.0120	240

T_r and T_j differential equations (1) are considered as models for primary and secondary loop.

Unscented Kalman Filter

The basic form of Unscented Kalman filter [6] for the identification of a process nonlinearity is given by

$$x(k)=[x(k-1) +\int_{k-1}^{k} F[x(\tau),u(k-1)]d\tau] + w(k) \qquad (15)$$

and

$$y(k)=H[x(k)] +v(k) \qquad (16)$$

In nonlinear dynamic systems, the true condition of the process is represented by an underlying state that cannot be directly observed, while external influences are introduced through input signals. The measurable output reflects the system's response, which depends on both internal behavior and external excitation. To realistically capture system behavior, uncertainty is incorporated through stochastic disturbances affecting both the evolution of the state and the measurement process. These disturbances are typically modeled with well-defined statistical characteristics to represent real-world variability. The relationship between variables is expressed using nonlinear functional mappings. One mapping describes how the internal state evolves over time, while another connects the state to observable outputs. This formulation allows the model to represent complex systems where linear assumptions are inadequate. For state estimation, the Unscented Kalman Filter utilizes the unscented transformation, a deterministic sampling technique that avoids explicit linearization. It selects a set of representative points around the current estimate and propagates them through the nonlinear functions. This process captures the impact of nonlinearity more effectively. Consequently, the transformed points preserve essential statistical properties, enabling accurate estimation of the system's mean and uncertainty, even in highly nonlinear environments.

$$x(k|k,0)=\hat{x}(k|k)$$

$$x(k|k,i) = \hat{x}(k|k) + (\sqrt{(L+\lambda)P(k|k)})_i$$

i=1, . . ., L

$$x(k|k,i) = \hat{x}(k|k) - (\sqrt{(L+\lambda)P(k|k)})_{i-L}$$

i=L+1 . . ., 2L

$$W^m(0) = \frac{\lambda}{L+\lambda}$$

$$W^c(0) = \frac{\lambda}{L+\lambda} + (1+\alpha^2+\beta)$$

$$\lambda = \alpha^2(L+k) - L$$

$$W^c(i) = W^m(i) = \frac{1}{2(L+\lambda)} \quad i=1, \ldots, 2L$$

k is a secondary scaling parameter, and it can be obtained from the equation k=3-L for gaussian distribution. α is a determining factor that the spread of sigma around $\hat{x}(k|k)$, which is chosen between 1e-4 to 1.[6,7] β is for prior knowledge distribution of $\hat{x}$ ad the optimum value for gaussian distribution[6] is 2. The 2L+1 sigma points have been derived from the state $\hat{x}(k|k)$ and covariance of the state vector $p(k|k)$, where L is the dimension of the state vector[6,7]. the set of sigma points are predicted in prediction step by propagating the sigma points in nonlinear differential equations[6,7].

$$x((k|k-1,i) = x((k-1|k-1,i) + \int_{k-i}^{k} F[x(\tau,i), u(k-1)]d \qquad i=0, \ldots,2L \qquad (17)$$

the prediction state estimates $\hat{x}(k|k-1)$ is got from predicted sigma points as[6,7]

$$\hat{x}(k|k) = \sum_{i=0}^{2L} W^m(i)\, x((k|k-1,i) \qquad (18)$$

The error covariance matrix $p(k|k-1)$ is got from the predicted sigma points as[6,7]

$$x((k|k-1,i) = \sum_{i=0}^{2L} W^c(i) x((k|k-1,i) - \hat{x}(k|k-1) * [x(k|k-1,i) - \hat{x}(k|k-1)]^T + Q \qquad (19)$$

the sigma points are redrawn by $\hat{x}(k|k-1)$ and $p(k|k-1)$ to add the effect of additive process noise and the predicted sigma points are passed through the nonlinear measurement equation to obtain the predicted measurement as[6,7]

$$\hat{y}(k|k-1) = \sum_{i=0}^{2L} W^m(i)\, H\,[x(k|k-1,i)] \qquad (20)$$

The covariance matrix of the innovations $p_{yy}(k)$ and the cross-covariance matrix between the predicted state estimate errors and innovations $p_{xy}(k)$ are computed as[6,7]

$$p_{yy}(k) = \sum_{i=0}^{2L} W^c(i)\, [H\,[x(k|k-1,i)] - \hat{y}(k|k-1)] * [H\,[x(k|k-1,i)] - \hat{y}(k|k-1)]^T + R \qquad (21)$$

$$p_{xy}(k) = \sum_{i=0}^{2L} W^c(i)\, [x\,[x(k|k-1,i)] - \hat{x}(k|k-1)] * [H\,[x(k|k-1,i)] - \hat{y}(k|k-1)]^T \qquad (22)$$

The residual is,

$$\gamma(k) = y(k) - \hat{y}(k|k-1) \qquad (23)$$

The Kalman matrix K(k) is identified as[6,7],

$$K(k) = p_{xy}(k) p_{yy}^{-1}(k) \qquad (24)$$

The updated state estimates $\hat{x}(k|k)$ are then obtained using the linear update equation as in the Kalman filter using the Equation 25.

$$p(k|k) = p(k|k-1) - K(k) * p_{yy}(k) K^T(k) \qquad (25)$$

Extended Kalman Filter

The Kalman filter solve the linear system.[6,7] The commonly used nonlinear filter is Extended Kalman filter. The basic Kalman filter is not highly applicable for nonlinear systems, because as a optimal filter its mathematics involves linearity.[6,7] It is overcome by EKF using linearized approximation, where the linearization happens around the current state estimate. The basic structure of EKF is given in Equation 16.

EKF performs recursive estimation of the mean and covariance of the state under maximum likelihood conditions.6,7 The function F can be used to calculate the prediction state from the previous state estimate and similarly function H can be used to calculate the predicted measurement from the predicted state.6,7 But F and H cannot be applied to the covariance directly. Instead, a Jacobian (a matrix of partial derivatives) is computed at each time step using current predicted state and evaluated. This action linearizes the nonlinear function around the current estimate.6,7 The predicted state estimates are,

$$\hat{x}((k|k-1,i) = \hat{x}((k-1|k-1) + \int_{k-1}^{k} F[x(\tau), u(k-1)]d\tau \quad (26)$$

The covariance matrix of estimation errors in the predicted state estimates is obtained as

$$\text{p}((k|k-1) = \emptyset(k)\ \text{p}((k-1|k-1)\emptyset(k)^T + Q \quad (27)$$

$\emptyset(k)$=exp[A(k)*T], A(k) is a Jacobian matrix of partial derivatives of F with respect to x and it is given by

$$\text{A(k)} = [\frac{\partial F}{\partial x}]_{[\hat{x}((k-1|k-1,u(k-1)]}$$

EKF measures covariances using the linear propagation by Eq. (27). The measurement prediction, assessment of innovation and covariance matrix of innovation[6,7] are calculated by,

$$\hat{y}((k|k-1) = H[\hat{x}((k|k-1)] \quad (28)$$

$$\gamma(k) = y(k) - \hat{y}((k|k-1) \quad (29)$$

$$\text{V(k)=C(k)P}((k|k-1)C(k)^T + R \quad (30)$$

C(k) is the Jacobian matrix of partial derivatives of H with respect to $\hat{x}$. [6,7] The Kalman gain is assessed by Equation (31).

$$\text{K(k)} = ((k|k-1)C(k)^T V^{-1}(k) \quad (31)$$

The state estimate updates and covariance matrix of identified errors in the updated state estimates are given in Equation (32) and Equation (33).[6,7]

$$\hat{x}((k|k) = \hat{y}((k|k-1) + K(k)\gamma(k) \quad (32)$$

$$P(k|k) = [I - K(k)C(k)]P(k|k-1) \quad (33)$$

UKF and EKF PID Control

The differential model Equation (1) – (9) gives the nonlinear dynamics of batch process. Two controllers are developed for the process, The PID controller parameters are estimated by UKF and EKF. For UKF and EKF parameter estimation refer Equation (15) – (33). In this part of work no reference model is considered, only the process future estimates determine the PID values. Table 2 gives the values of UKF PID and EKF PID.

Table 2: UKF and EKF PID parameters

Controller		K_p	K_i	K_d
UKF PID	Primary loop	150	0.5	20
	Secondary loop	50	0.2	10
EKF PID	Primary loop	0.91004	0.17999	0.01
	Secondary loop	0.99065	0.0018663	0.032538

Nonlinear Model-Based Controller

NMBC is the design of model-based controller for nonlinear system employes nonlinear model rather than N-number of linear models .[1,5] The blueprint of NMBC is given in fig. 3.[5] Consider the nonlinear system represented by the state and measurement equation as[5]

$$\text{x(k)=[x(k-1)} + \int_{k-1}^{k} F[x(\tau), u(k-1)]d\tau] \quad (34)$$

$$\text{y(k)=Cx(k)} \quad (35)$$

where, x(k)$\in R^n$ is the state variables, u(k) $\in R$ is the manipulated input variable, y(k) $\in R$ is a measured output variable. The NMBC formulation for a system is discussed in upcoming steps.[5]

step-1: determination of model state (x_m) by answering the nonlinear equation

$$x_m(k) = [x_m\ (\text{k-1}) + \int_{k-1}^{k} F[x_m(\tau), u(k-1)]d\tau] \quad (36)$$

Step-2: the value of $u_P(k)$ is determined by Equation (37).

$$F[x_m(k), u_P(k)] = 0 \quad (37)$$

Step-3: compute the value of $u_c(k)$ by Equation (38).

$$u_c(k) = K_c e(k) = K_c[y_{sp}(k) - y(k)] \quad (38)$$

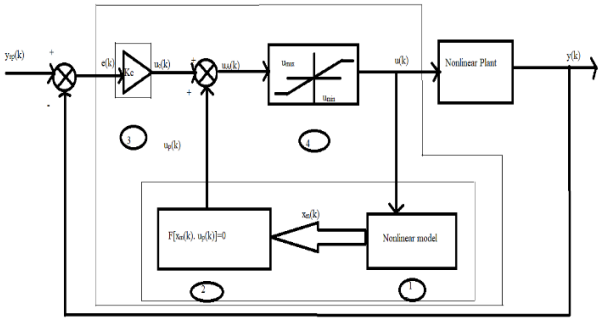

Fig. 3: Schematic Diagram of Nonlinear Model Based Control Scheme

Where, K_c is controller gain, in this UKF and EKF are used to get the optimized value of K_c by estimating optimal future outputs.[1,5] y_{sp} and y are setpoint and measured process variable. Then $u_A(k)$ is calculated by

$$u_A(k) = u_P(k) + u_c(k) = u_P(k) + K_c[y_{sp}(k) - y(k)] \quad (39)$$

Step-4: if the calculated value of $u_A(k)$ is outside the feasible region, then it is projected to the boundary to obtain the constrained value of controller output u(k) is given by,

$$\text{u(k)} = u_{min} \leq u_A(k) \leq u_{max} \quad (40)$$

u_{max} and u_{min} are the limits associated with the manipulated variable. It is clear u(k) is given as an input to the nonlinear system.

UKF and EKF NMBC Control

NMBC control parameters are estimated by Ukf and Ekf methods. Refer Equation (33) – (40) for NMBC formulation.[1,5] Here NARX model of T_r is used as reference model for NMBC and Ukf, Ekf estimates the future process outputs, for this refer Equation (15) – (33).[6] Based on the future estimate of the process and reference model output, NMBC controller parameters are estimated and updated. Table 3 gives details about the NMBC control parameters involved in simulation study.

Table 3: UKF and EKF NMBC Control Parameters

Parameters	UKF NMBC	EKF NMBC
Initial State Estimate	$[4.5\times10^{-5}, 0.7034, 55, 36.8]^T$	$[4.5\times10^{-5}, 0.7034, 55, 36.8]^T$
NMBC gain K_c	2	2
C_p	[0, 0, 0, 1]	[0, 0, 0, 1]
Parameters	**UKF NMBC**	**EKF NMBC**
NMPC prediction and control Horizon	5 and 3	5 and 3
W_e , W_u	5 and 0.5	5 and 0.5
$P(0\|0)$	diag ([1e-6, 1e-4, 1, 1])	diag([1e-6, 1e-4, 1, 1]
Q_k	diag([1e-10, 1e-6, 0.01, 0.01])	diag([1e-10, 1e-6, 0.01, 0.01])
R_k	diag([0.1, 0.1])	diag([0.1, 0.1])
C_m	[0 0 1 0 0 0 0 1]	[0 0 1 0 0 0 0 1]
Tuning parameters	$\alpha = 0.001, \beta = 2, K = 0$	$\alpha = 0.001, \beta = 2, K = 0$

Performance Index

Control effort is taken as performance index to analyze the success of the developed control strategies. There are different types of methods are there to calculate control effort, they are absolute variation method, quadratic variation method and control energy method. The physical interpretation of control effort is the total absolute change in the control signal over the time horizon. Here we calculate control effort for total variation of control signal.[6] Since we measure the smoothness of the control signal, absolute variation method of control effort calculation is recommended,

its unit is in J/K. the control effort is given by,

$$\text{Control effort} = \sum_{k-2}^{N} |u(k) - u(k-1)| \quad (41)$$

Where, k is the point of time, u is the controller output, that is signal from the Unscented Kalman Filter based Nonlinear model-based controller and Extended Kalman Filter based Nonlinear model-based controller

Results and Discussion

The closed loop response of reactor temperature of normal Cascade control, Unscented Kalman Filter PID control and Extended Kalman Filter PID control, Unscented Kalman Filter based Nonlinear model-based control and Extended Kalman Filter based Nonlinear model-based control is shown in fig. 4 to 7. From fig 4 conventional PID controller unable to take actions to track the reference input, this is because the system is highly nonlinear, but the controller is linear. This makes the controller inefficient, the controller response signifies that there is no coolant flow, so the process remains in 40℃. To overcome this inefficiency, controller should be developed very rigidly to take control actions to track the reference. So, the PID control parameters are estimated by Unscented Kalman Filter and Extended Kalman Filter techniques.

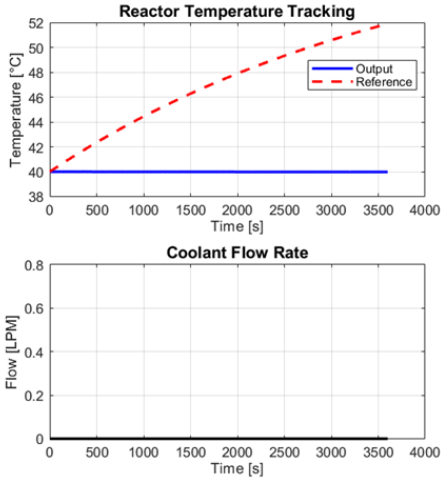

Fig. 4: Conventional Cascade Control Response

The Ukf PID and Ekf PID response are as follows:

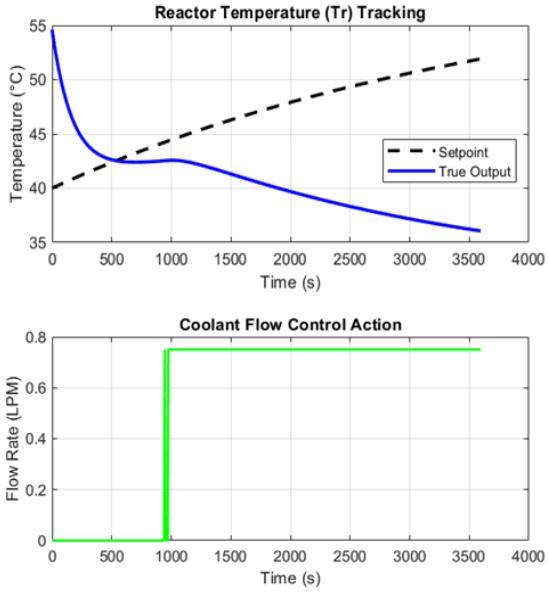

Fig. 5: UKF PID Controller Response

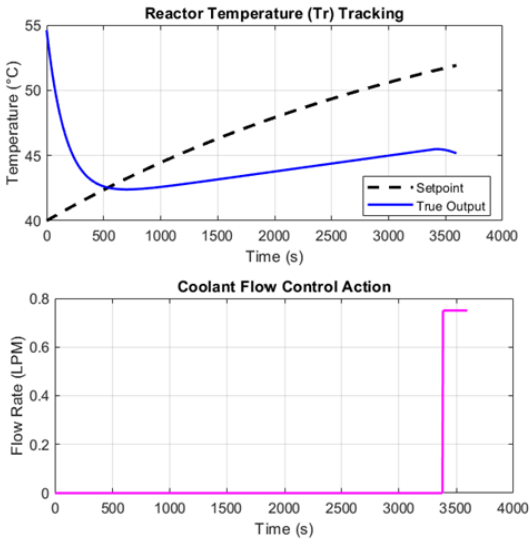

Fig. 6: EKF PID Controller Response

From the response we signified that Unscented Kalman Filter PID and Extended Kalman Filter PID trying to track the reference. Unscented Kalman Filter PID almost makes maximum coolant flow while Extended Kalman Filter PID makes maximum coolant flow at end of the batch time. But both controllers unable to track the reference. Unscented Kalman Filter Nonlinear Model Based Control and Extended Kalman Filter based Nonlinear Model based Control response signifies that, these two controllers able to track the reference. But Ukf Nmbc outperforms Ekf Nmbc by control Effort. This is because Ekf Nmbc makes local linearization of Jacobian matrix. Table 4 gives the control effort values and Final covariance matrices of Ukf Nmbc and Ekf Nmbc. The performance indices considered in this work is control effort. The control effort values of Ukf Nmbc and Ekf Nmbc are given in table 4.

The Ukf Nmbc and Ekf Nmbc response are as follows:

Comparison response of Ukf Nmbc and Ekf Nmbc are shown in fig. 7.

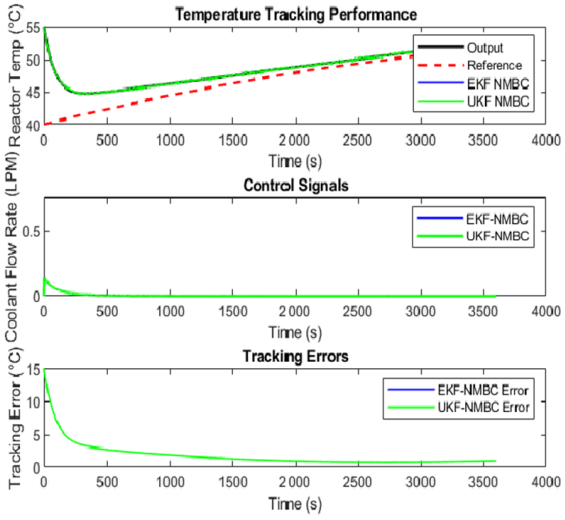

Fig. 7: UKF NMBC and EKF NMBC Controllers' Response

Ukf Nmbc and Ekf Nmbc response signifies that, these two controllers able to track the reference. But Ukf Nmbc outperforms Ekf Nmbc. This is because Ekf Nmbc makes local linearization of Jacobian matrix.[6] Table 4 gives the control effort values and Final covariance matrices of Ukf Nmbc and Ekf Nmbc. The performance indices considered in this work is control effort. The control effort values of Ukf Nmbc and Ekf Nmbc are given in table 4.

Table 4: Control Effort and Covariance Matrices

Controller	Control Effort J/K	Final Covariance Matrix
Ukf Nmbc	36.8030	0.0000 −0.0001 0.0000 − 0.0000 −0.0001 0.0824 −0.0005 0.0000 0.0000 −0.0005 0.0361 0.0005 -0.0000 0.0000 0.0005 0.0370
Ekf Nmbc	36.6654	0.0000 −0.0001 0.0000 − 0.0000 −0.0001 0.0945 −0.0007 0.0000 0.0000 −0.0007 0.0263 0.0004 -0.0000 0.0000 0.0004 0.0270

Conclusion

This work addresses A successful implementation of Conventional PID, Ukf PID, Ekf PID, Ukf Nmbc, and Ekf Nmbc for the batch polymerization reactor. Based on the literature NARX model of reactor temperature is chosen as reference model for nonlinear model-based control scheme. All the controller response signifies that linear control for nonlinear process is not successful and efficient, that the Conventional PID control scheme developed is unable to track the reactor temperature profile, this is very clear from the conventional PID control scheme response. In other hand, Even Ukf PID and Ekf PID controller also unable to track the reference, this is proven by the responses of the control schemes. Only the Ukf Nmbc and Ekf Nmbc makes optimal reference tracking of reactor temperature profile, in that Ukf Nmbc is most successful and efficient for the process based on the control effort value. In other hand Ekf Nmbc developed for comparative analysis gives better result, but the control effort value is slightly less when compared with Ukf Nmbc. This simulation study strongly suggests that Ukf strategies is more applicable for a nonlinear batch polymerization process. In future these results will be employed in real time plant.

Appendix

Nomenclature

Parameters involved in the process are[1,2],

[I]	initiator concentration	[M]	monomer concentration
α, β	heat loss coefficients	ΔH_p	heat of polymerization
ε, θ	reaction constants	A	area of heat transfer
C_{p1}	specific heat of the solvent	C_{p2}	specific heat of the initiator
C_{p3}	specific heat of the monomer	C_{p4}	specific heat of the polymer
C_{p5}	specific heat of the stirrer	C_{p6}	specific heat of the reactor wall
C_{p7}	specific heat of the coolant fluid	C_{p8}	specific heat of the cooling coil
C_{pc}	specific heat of the coolant	d	diameter of the stirrer blades
E_d	dissociation enthalpy	E_p	polymerization enthalpy
F_c	coolant flow rate	m_1	mass of the solvent(water)
m_2	number of moles of initiator	m_3	number of moles of monomer
m_4	number of moles of polymer	m_5	mass of stirrer
m6	mass of reactor vessel	m_7	mass of the coolant fluid
m8	mass of cooling coil	n	rotational speed of the stirrer
P_0	power number	Q_h	heat added to the reactor
Q_R	heat due to the reaction	Q_s	heat added by the stirrer
T_c	coolant temperature	T_j	jacket temperature
T_{amb}	ambient temperature	U	overall heat transfer coefficient
V	volume of the reaction mixture	A_d	dissociation constant
A_p	polymerization constant	ρ	density of the reaction mixture

Parameter Values

Reactor parameter values and abbreviations are taken from literature[1,2].

$A = 4.4\times10^{16}$ s-1	$A_p = 2.833\times10^{9}$ L0.75mol-0.75s-1
$E_d = 140.06\times10^{3}$ J	$E_p = 7.0711\times10^{4}$
R = 8.3145 J/ (mol K)	ε = 0.5
θ = 1.25	V = 0.5 L
$\Delta H_p = -82.2\times10^{3}$ J/mol	$P_0 = 10.72035$
$\rho = 1000.05\times10^{3}$/m3	n = 200 rpm=3.33rps
d = 0.05m	α = 1.0003W°C^(-β)
β = 0.001845	m_1=450g
m_2(initial)=4.5×10^{-5}mol	m_3(initial)=0.7.34mol

m_4(initial)=0 mol	m_5=220g
m_6=7200g	m_7=18g
m_8=240g	C_{p1}=4.184 J/g°C
C_{p2}=187 J/mol °C	C_{p3}=110.58 J/mol °C
C_{p4}=84.95 J/mol° C	C_{p5}=0.49 J/g°C
C_{p6}=0.49 J/g°C	C_{p7}=4.184 J/g°C
C_{p8}=0.49 J/g°C	T_{amb}=27°C

References

Yadav, E. S., Shettigar J, P., Poojary, S., Chokkadi, S., Jeppu, G., & Indiran, T. (2021). Data-driven modeling of a pilot plant batch reactor and validation of a nonlinear model predictive controller for dynamic temperature profile tracking. *ACS omega*, *6*(26), 16714-16721. https://doi.org/10.1021/acsomega.1c00087

Fathima Sapna, P. (2021). Load Frequency Control of Thermal Power System by using Extended PI & FLC. *International Academic Journal of Innovative Research, 8*(2), 01–05. https://doi.org/10.9756/IAJIR/V8I2/IAJIR0803

Mahadi, M., Ballal, T., Moinuddin, M., & Al-Saggaf, U. M. (2022). A recursive least-squares with a time-varying regularization parameter. *Applied Sciences*, *12*(4), 2077. https://doi.org/10.3390/app12042077

Arasu, S. K., Panda, A., & Prakash, J. (2016). Experimental validation of a Nonlinear Model based Control scheme on the Variable area tank process. *IFAC-PapersOnLine*, *49*(1), 30-34. https://doi.org/10.1016/j.ifacol.2016.03.024

Subramaniam, K. (2025). Design Optimization of Thermal Systems Using the Nusselt Number Correlation Approach. *Association Journal of Interdisciplinary Technics in Engineering Mechanics*, *3*(4), 20-27.

Prakash, J., Patwardhan, S. C., & Shah, S. L. (2010). State estimation and nonlinear predictive control of autonomous hybrid system using derivative free state estimators. *Journal of process control*, *20*(7), 787-799. https://doi.org/10.1016/j.jprocont.2010.04.001

Chitralekha, S. B., Prakash, J., Raghavan, H., Gopaluni, R. B., & Shah, S. L. (2009). Comparison of expectation-maximization based parameter estimation using particle filter, unscented and extended Kalman filtering techniques. *IFAC Proceedings Volumes*, *42*(10), 804-809.

Prakash, J., Patwardhan, S. C., & Shah, S. L. (2010). Constrained nonlinear state estimation using ensemble Kalman filters. *Industrial & Engineering Chemistry Research*, *49*(5), 2242-2253

Serrano, F., & Rossell, J. M. (2019). Anti-windup control of nonlinear cascade systems with particle swarm optimization parameter tuning. In *Advances in Control, Signal Processing and Energy Systems: Select Proceedings of CSPES 2018* (pp. 3-16). Singapore: Springer Singapore. https://doi.org/10.1007/978-981-32-9346-5_1

Bae, J. E., Kim, K. H., Chu, S. C., Heo, J., Lim, S., & Sung, S. W. (2020). Development of an antiwindup technique for a cascade control system. *ACS omega*, *5*(50), 32597-32607. https://doi.org/10.1021/acsomega.0c04927

Van De Geer, S. A. (2005). Least squares estimation. *Encyclopedia of statistics in behavioral science*,2, 1041–1045. https://doi.org/10.1002/0470013192.bsa199

Balakrishnan, M., Rajendran, V., Prajwal, S. J., & Indiran, T. (2023). Neural network-based Hammerstein model identification of a lab-scale batch reactor. *ACS omega*, *9*(1), 1762-1769. https://doi.org/10.1021/acsomega.3c05406

Mehrani, M. J., Bagherzadeh, F., Zheng, M., Kowal, P., Sobotka, D., & Mąkinia, J. (2022). Application of a hybrid mechanistic/machine learning model for prediction of nitrous oxide (N2O) production in a nitrifying sequencing batch reactor. *Process Safety and Environmental Protection*, *162*, 1015-1024. https://doi.org/10.1016/j.psep.2022.04.058

Rahrooh, A., & Shepard, S. (2009). Identification of nonlinear systems using NARMAX model. *Nonlinear Analysis: Theory, Methods & Applications*, *71*(12), e1198-e1202. https://doi.org/10.1016/j.na.2009.01.150

Kumar, S., Prakash, J., & Kanagasabapathy, P. (2011). A critical evaluation and experimental verification of Extended Kalman Filter, Unscented Kalman Filter and Neural State Filter for state estimation of three phase induction motor. *Applied Soft Computing*, *11*(3), 3199-3208. https://doi.org/10.1016/j.asoc.2010.12.022