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System Identification of Batch Polymerization Reactor by Means of Estimator Algorithms and Performance Analysis of Autoregressive Exogenous Models

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Abstract

Batch reactor is an irreplaceable process of many industries. An essential task in any industrial process is model identification. Any mathematical model, including transfer functions, state spaces, and differential equations, can be used to depict a process. In some cases, due to our limited knowledge of the model parameters, the process couldn't be represented mathematically. In these situations, instead of white and gray box technique the black box model technique has been used, in which the process input and output data are subjected to various estimation methods for the model parameter identification. Here, least mean square and recursive least square algorithms are chosen as estimators. This work concentrates on ARX, NARX, and NARMAX model identification of reactor temperature T_r of batch process. The reactor temperature data is collected by solving process differential equation. Those data are subjected to estimation algorithms to find the ARX, NARX, and NARMAX model parameters. Identified model outputs are validated with process reactor temperature T_r data. The best model and estimation algorithm are highlighted from the computational study for future work.

Keywords: Reactor Temperature T_r, Jacket Temperature T_j, Least Mean Square LMS, Recursive Least Square RLS, Auto Regressive Exogenous Arx Model, I Initiator Ammonium Persulphate Concentration, M Monomer Concentration.

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Introduction

Batch reactor is a highly nonlinear process, the reaction between a input materials take place in a protected sealed chamber, which means the process does not have continues input and output (Yadav et al., 2021; Shettigar et al., 2021). Instead, the feed is placed inside the reactor for the specific time to produce the final product. The major goal is to regulate the reactor and jacket temperatures to produce the desired product. Coolant that circulates around the reactor's jacket helps indirectly regulate the reactor temperature, to produce the final output. Batch reactor modelling and control is very challenging work. Many developed linear and nonlinear model with random nonlinear profiles (Yadav et al., 2021; Shettigar et al., 2021; Cott & Macchietto, 1989).

This effort entails simulating the batch reactor temperature profile for monomer to polymer conversion. The reactor differential equation model and lms-based data driven model were created (Yadav et al., 2021; Shettigar et al., 2021). this work focuses on least mean square-based model identification of ARX and NARX models along with NARMAX model. In addition, this work suggests recursive least square-based model parameter estimation to test the effectiveness of the better estimation technique. The open loop data of the differential equation is taken into consideration for least mean square and recursive least square algorithms, which constructs ARX, NARX, NARMAX models (Mahadi et al., 2022; Yadav et al., 2021; Shettigar et al., 2021).

The non-linear differential equations of I, M, Tr, Tj are considered, because it is safe and secure for us to conduct open loop test in mathematical model, instead of real time plant. Most precisely the chosen differential equations are highly equivalent to the real process, which is confirmed by the literature (Yadav et al., 2021; Shettigar et al., 2021). The differential equations system dynamics are chosen from the literature (Yadav et al., 2021; Shettigar et al., 2021). The system identification models like ARX, NARX (Yadav et al., 2021; Shettigar et al., 2021). and NARMAX (Alireza Rahrooh et al., 2009) were identified for nonlinear batch reactor temperature profiles.

Least square estimation and recursive least square, both fixed regularization parameter and non-fixed regularization parameter were developed for nonlinear processes (Mahadi et al., 2022; Van de Geer, 2005). based on above work, least mean square and recursive least square algorithms of fixed regularization parameter are developed for the batch polymerization process. To develop a perfect reactor temperature profile model, Modeling of lipase catalyzed esterification process is studied (Zulkeflee et al., 2021). Autoregressive exogenous models were developed for lipase catalyzed esterification process (Zulkeflee et al., 2021). Literature gives details about Batch reactor modeling and optimal control for different objective functions (Senthil & Sundaramoorthy, 2018). this computational study concentrates on developing best fit autoregressive exogenous model for reactor temperature T_r of batch process by least mean square and recursive least square estimation techniques.

Batch Reactor

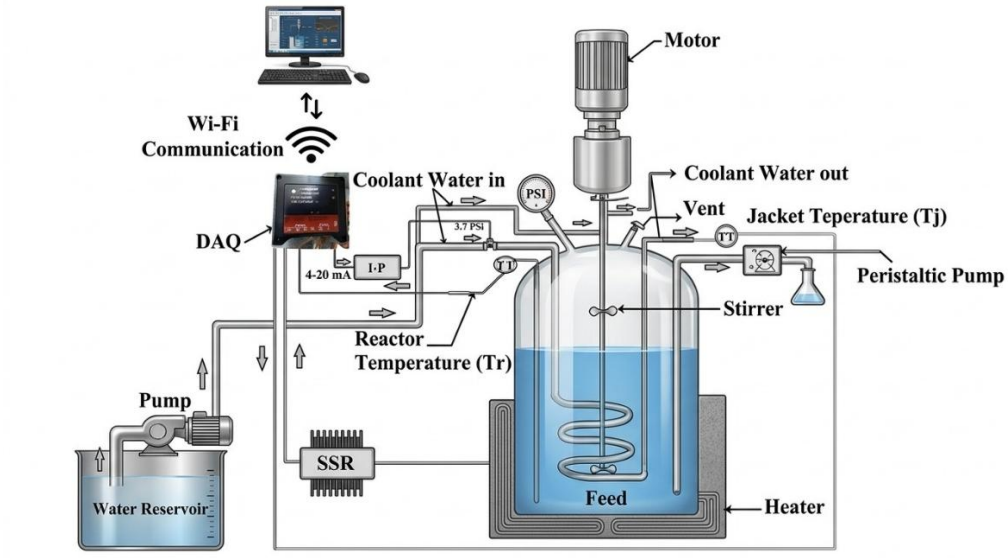

Fig. 1: Batch Polymerization Reactor

The fig. 1 is the schematic diagram of the monomer to polymer batch reactor (Shettigar et al., 2021), which comprises

of reactor chamber with agitator run by an electric motor. The sump has coolant liquid circulates around the reactor and the entire reactor is placed above the heater. This setup consists of temperature sensors, flow sensors, pressure sensors, which are all communicates to the pc through DAQ.

Dimensions

The dimensions of batch polymerization reaction (Yadav et al., 2021; Shettigar et al., 2021) are,

Inner diameter of the reactor is 101.6 mm

Outer diameter of the reactor is 197 mm

Inner height of the reactor is 169 mm

External height of the reactor is 183 mm

Length of the coolant coil is 1340 mm

Outer diameter of the coolant coil is 6.35 mm

Area of the batch reactor (A) is 0.06824193 m^2

Coefficient of heat transfer (U) is 500 $Wm^{-2}\ K^{-1}$

Heater wattage is 1500 W (maximum)

Pressure range is 100 bar (maximum)

Control valve pneumatic (air to close type 3−15 psi)

Agitator 1200 rpm (maximum)

Differential Equation of Process

The differential equations model of batch process is given in equation 1 to equation 9 (Shettigar et al., 2021).

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

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

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

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

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

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

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

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

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

Initiator, monomer concentration, reaction temperature, reaction speed, and polymerization are the variables that affect monomer conversion (Yadav et al., 2021; Shettigar et al., 2021). The reason behind the energy absorbed or released in the batch reactor are, heating of monomer feed inside the reactor chamber, coolant circulates in the jacket and the heat produced by exothermic reaction (Yadav et al., 2021; Shettigar et al., 2021). The reaction heat is calculated by reactors heat capacity and the mass of the feed (Shettigar et al., 2021). The differential equation of the reactor temperature T_r is given in equation 3 (Shettigar et al., 2021).

During the heating phase, the temperature in the jacket is maintained at a constant level that in basic room temperature, and jacket dynamics are crucial in batch process control (Yadav et al., 2021; Shettigar et al., 2021). By using cooling system, that have been added to the cascade control method, it is possible to effectively regulate jacket dynamics by adjusting the temperature of the jacket coolant inlet (Yadav et al., 2021; Shettigar et al., 2021). The jacket temperature is given in equation 4 (Shettigar et al., 2021). Heat due to reaction of chemical components inside the rector Q_R given in equation 5, at the time of rection heat given by the stirrer Q_s is given by equation 6, heat loss during the reaction

Q_{loss} is given by equation 7, Product of Specific heat (solvent, initiator, monomer, polymer, stirrer, reactor wall) and mass (solvent, initiator, monomer, polymer, stirrer, reactor wall) is given by equation 8, then product of Specific heat (coolant fluid and cooling coil) and mass (coolant fluid and cooling coil) given by equation 9 (Shettigar et al., 2021).

The non-feedback test is conducted by the following considerations, the embryonic values of reactor temperature T_r and jacket temperature T_j are taken as 55° Cand 36.8 ° C (Yadav et al., 2021; Shettigar et al., 2021), the coolant flow rate is maintained as 0 and 0.75 Lpm, assume coolant temperature and ambient temperature are equal (Yadav et al., 2021; Shettigar et al., 2021). The reaction mixture values are selected to be 500mL of 10% monomer and 5mL of 0.009 mol/L and consider $[Q_{h\,Fc}] = [60\ 70]$ to reach initial steady state and then by step change of [60 50] (Yadav et al., 2021; Shettigar et al., 2021; Palanki et al., 1993).

System Identification

Modelling of ARX, NARX, NARMAX for reactor temperature has been carried out in this work. General structure of ARX is given by the equation 10 (Yadav et al., 2021; Shettigar et al., 2021). the input, output and error orders are n_u=1, n_y=2 and n_e=2 (Shettigar et al., 2021).

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

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 effortless 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 rationalize the model training (Yadav et al., 2021 & Shettigar et al., 2021). NARX model is given in equation 11 (Yadav et al., 2021; Shettigar et al., 2021)

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

NARMAX model includes past errors along with current prediction errors. Here also nonlinear function used for mapping of past input, outputs to current output. NARMAX model gives improved results for complex systems. Polynomial nonlinear function is used in NARX and NARMAX models (Rahrooh & Shepard, 2009). NARMAX model is given in equation 12 (Rahrooh & Shepard, 2009).

$$y(t)_{NARX} = \sum_{i=0}^{n_u} a(i)(u(t-i) + \sum_{j=1}^{n_y} b(j)y(t-j) + \sum_{k=1}^{n_e} d(k)e(t-k) + \sum_{i=0}^{n_u}\sum_{j=1}^{n_u} A(i,j)u(t-i)u(t-j) + \sum_{i=1}^{n_y}\sum_{j=i}^{n_y} B(i,j)y(t-i)y(t-j) + \sum_{i=0}^{n_u}\sum_{j=1}^{n_y} C(i,j)u(t-i)y(t-j) + \sum_{i=o}^{n_u}\sum_{k=1}^{n_e} D(i,k)u(t-i)e(t-k) + \sum_{j=1}^{n_y}\sum_{k=1}^{n_y} E(j,k)y(t-j)e(t-k) + \sum_{k=1}^{n_e}\sum_{l=k}^{n_e} F(k,l)e(t-k)e(t-l) \quad (12)$$

Where a(i), A (i, j) are the linear and nonlinear coefficients for exogenous input terms, b(j), B (i, j) are the coefficients of linear and nonlinear autoregressive terms, C (i, j) is the coefficients of the nonlinear cross terms (Yadav et al., 2021; Shettigar et al., 2021). D (i, k), E (j, k), and F (k, l) are coefficients are error terms (Yadav et al., 2021; Shettigar et al., 2021; Rahrooh & Shepard, 2009).

Parameter Estimation

Parameters of ARX, NARX and NARMAX models are estimated by Least mean Square (Yadav et al., 2021; Shettigar et al., 2021; Rahrooh & Shepard, 2009). and Recursive Least Square techniques (Mahadi et al., 2022; Van de Geer, 2005).

Least Mean Square Estimation

Least mean square is estimation technique, which is used to estimate the model parameters (Yadav et al., 2021; Mahadi et al., 2022). The basic structure of lms is given in equation 13.

$$y = Ax + z \quad (13)$$

Where, vector x∈ $R^{n\times1}$ is going to be estimated and vector y∈ $R^{m\times1}$is sample vector, A∈ $R^{m\times n}$ is a data set and z∈ $R^{m\times1}$ is a normal random vector (Van de Geer, 2005). The lms algorithm solves the unconstrained minimization problem (Van de Geer, 2005),

$$min_{\hat{x}} \|y - A\hat{x}\| \frac{2}{2} \quad (14)$$

lms is adaptive filter that works on gradient descent approach to minimize the squared error loss 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 15.

$$x_{ls}=(A^TA)^{-1}A^Ty \quad (15)$$

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.

Recursive Least Square Estimation

The dimension of y and A is m, such that those can be denoted as y_m and A_m. the observation vector entries are mentioned as d_i and the individual row of A is U_i^T. while the estimation processes, the dimension of A_m and y_m increases by 1 and those can be written as A_{m+1}, y_{m+1}. They are written as follows (Van de Geer, 2005; Mahadi et al., 2022),

$$y_{m+1}=\begin{bmatrix} y_m \\ d_{m+1} \end{bmatrix} \quad (16)$$

$$A_{m+1}=\begin{bmatrix} A_m \\ U_{m+1}^T \end{bmatrix} \quad (17)$$

Where d_{m+1} is new sampled data and U_{m+1}^T is new row of A (Van de Geer, 2005). here m can be mentioned as time index as well (Van de Geer, 2005; Mahadi et al., 2022). The model parameter estimate x of m dimension is given by equation 18.

$$x_m=(A_m^TA_m+\gamma I_n)^{-1}A_m^Ty_m \quad (18)$$

The time updates update of x_{m+1} is given by,

$$x_{m+1}=(A_{m+1}^TA_{m+1}+\gamma I_n)^{-1}A_{m+1}^Ty_{m+1} \quad (19)$$

γ is a regularization parameter, here fixed regularization parameter method of rls is implemented (Mahadi et al., 2022) its value varies between 0 to1, I is an identical matrix of order n. the recursive formula of estimates for before and after update is given by equation 20 and 21.

$$x_m=P_mA_m^Ty_m \quad (20)$$

$$x_{m+1}=P_{m+1}A_{m+1}^Ty_{m+1} \quad (21)$$

Were

$$P_m \triangleq (A_m^TA_m+\gamma I_n)^{-1} \quad (22)$$

$$P_{m+1} \triangleq (A_m^T+1A_{m+1}+\gamma I_n)^{-1} \quad (23)$$

$P_0=\frac{1}{\gamma}I_n$ is an initial condition and P_m can be viewed as inverse of scaled regularized covariance matrix (Mahadi et al., 2022). So p_{m+1} is written as follows,

$$P_{m+1}=(P_m^{-1}+U_{m+1}U_{m+1}^T)^{-1} \quad (24)$$

Using matrix inversion lemma, P_{m+1} becomes,

$$P_{m+1}=P_m-\frac{P_mU_m+1U_{m+1}^TP_m}{1+U_{m+1}^TP_mU_{m+1}} \quad (25)$$

The updated estimates can get by substituting Equation 25 in equation 21.

$$x_{m+1}=x_m+\frac{P_mU_m+1}{1+U_{m+1}^TP_mU_{m+1}}[d_{m+1}-U_{m+1}^Tx_m] \quad (26)$$

The initial x_0 is taken as 0 and P0 is $\frac{1}{\gamma_0}$I based on literature (Mahadi et al., 2022). The algorithm calculates P_{m+1} and x_{m+1} for new sample dm+1 and new row U_{m+1}^T (Van de Geer, 2005).

Result and Discussion

The differential equation of the batch reactor is considered as process for the simulation work. By solving the equations, the data required for developing system identification models are collected. The non-feedback differential

equation response of the process is shown in fig. 2.

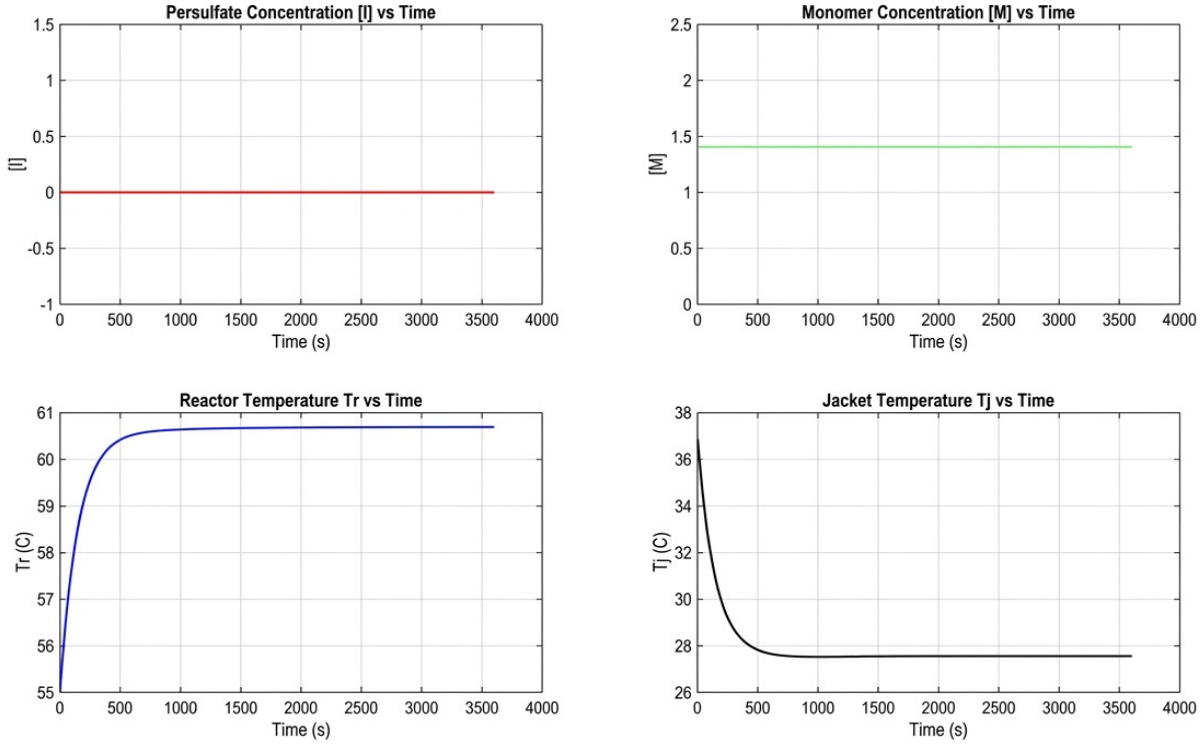

Fig. 2: The Non-Feedback Response of Differential Equations of Batch Reactor Comprises of Persulphate, Monomer Concentration, Reactor Temperature and Jacket Temperature

The data collected by solving process differential equations are subjected to both least square and recursive least square algorithms. The ARX, NARX and NARMAX model parameters are estimated individually by both the algorithms. The model coefficient a, b, A, B, C, D, E, F are named as same as from previous work (Yadav et al., 2021; Rahrooh & Shepard, 2009). the lms estimated model parameters for reactor temperature T_{rARX} are, a (1) = -0.1348, b (1) =0.1850 and b (2) =0.2197. the same way lms estimated model parameters of T_{rNARX} are, a (0) = 0, a (1) =0, b (1) = 0, b (2) = 0, A (0,1) = -0.0822, A (1,1) = 0.0929, B (1,1) = 0.0953, B (1,2) = 0.0540, B (2,2) = -0.0606, C (0,1) = -0.0802, C (0,2) = -0.1035, C (1,1) = 0.0197, C (1,2) = 0.0290 and for $T_{rNARMAX}$, a (0) = 0, a (1) =0, b (1) = 0, b (2) = 0, d (1) =0, d (2) =0, A (0,1) = -0..0585, A (1,1) = 0.0549, B (1,1) = 0.0561, B (1,2) = 0.0294, B (2,2) = 0.0037, C (0,1) = -0.0010, C (0,2) = -0.0068, C (1,1) = -0.0082, C (1,2) = -0.0042, D (0,1) = -0.0127, D (0,2) = -0.0136, D (1,1) = 0.0111, D (2,2) = 0.0119, E (1,1) = 0.0087, E (1,2) = 0.0098, E (2,1) = 0.0120, E (2,2) = 0.0120, F (1,1) = 0.0115, F (1,2) = 0.0469, F (2,1) = 0.0459, F (2,2) = 0.

The rls estimated model parameters for reactor temperature T_{rARX} are, a (1) = -0.0033, b (1) = 1.7639 and b (2) = -0796. the same way rls estimated model parameters of T_{rNARX} are, a (0) = 0, a (1) =0, b (1) = 0, b (2) = 0, A (0,1) = -0.0884, A (1,1) = 0.6152, B (1,1) = 0.4388, B (1,2) = 0.0369, B (2,2) = 0.1156, C (0,1) = -0.0453, C (0,2) = 0.1037, C (1,1) = 0.0055, C (1,2) = -0.1145 and for $T_{rNARMAX}$, a (0) = 0, a (1) =0, b (1) = 0, b (2) = 0, d (1) =0, d (2) =0, A (0,1) = -0.2746, A (1,1) = -0.5566, B (1,1) = -0.6415, B (1,2) = -0.7706, B (2,2) = 0.2353, C (0,1) = 0.3283, C (0,2) = -0.9445, C (1,1) = -0.3212, C (1,2) = -1.3326, D (0,1) = -0.4452, D (0,2) = -1.5755, D (1,1) = -0.5754, D (2,2) = -1.2289, E (1,1) = 1.3837, E (1,2) = -0.3070, E (2,1) = 0.0127, E (2,2) = 0.0127, F (1,1) =0.0120, F (1,2) = 1.3504, F (2,1) = 0.7727, F (2,2) = 0.

Least mean square technique estimated model parameters based on whole dataset, which makes higher computational time and less accuracy for complex systems, while in other hand recursive least square estimated best fit model parameters by every newly observed data point, that at every time instant x_{m+1} is updated until the best fit model parameters are identified. rls can work on minimum data obtained, which gives perfect fitting parameters for models (Mahadi et al., 2022). Fig. 3 and fig. 4 shows the comparative analysis of ARX, NARX and NARMAX models identified by least mean square and recursive least square techniques. From the responses recursive least square based models are best fit with the actual process reactor temperature T_r output. This is because least square estimates the

model parameters is an elementary method that, the data set length decides the rightness of the models estimated (Yadav et al., 2021). but in recursive least square, irrespective of data set length, the estimated models give best responses (Van de Geer, 2005).

In other hand, NARX and NARMAX models estimated by recursive least square makes perfect fit, when compared to ARX model. But NARMAX model shows some uncertainty in initial transient time, this is because model complexity. But NARX model accurately fitted with the reactor temperature T_r data. In literature NARX model is identified by least mean square technique (Yadav et al., 2021; Shettigar et al., 2021). The identified NARX model by recursive least square outperforms the previous NARX model proposed in literature (Yadav et al., 2021; Shettigar et al., 2021)

This is proven by the performance indices consider in this work. Here mean square error (MSE) (Yadav et al., 2021) and root mean square error (RMSE) (Yadav et al., 2021) are considered for performance analysis of the identified models (Yadav et al., 2021). Equation 27 and 28 represent the error criterions (Yadav et al., 2021).

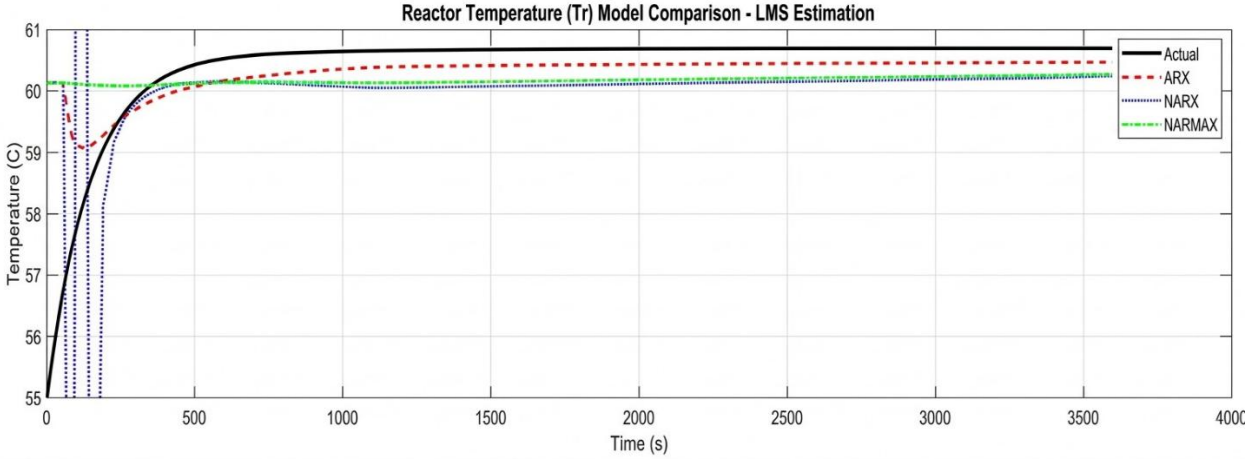

Fig. 3: Least Mean Square Estimated ARX, NARX and NARMAX Model Responses Compared with Actual Reactor Temperature T_r Data

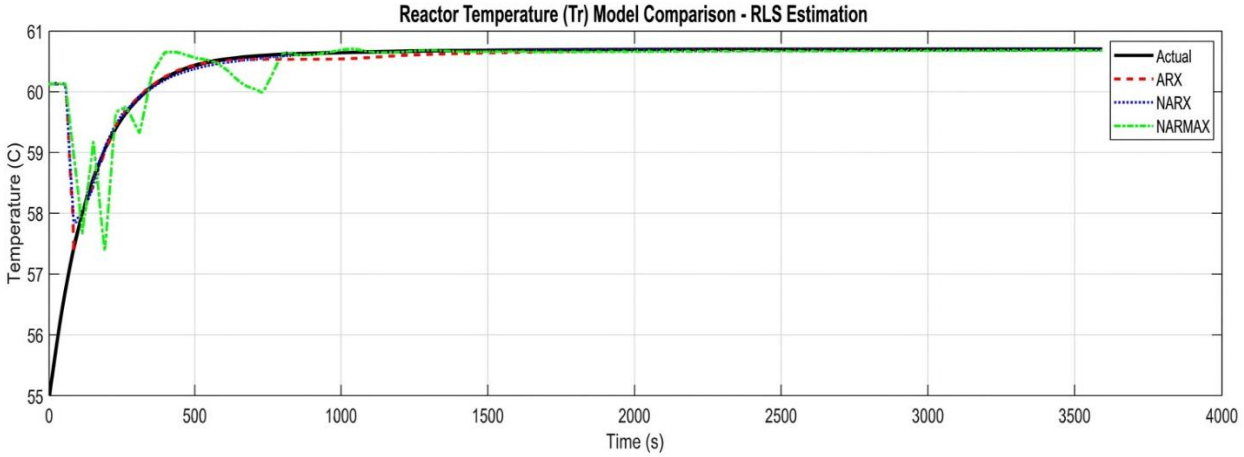

Fig. 4: Recursive Least Square Estimated ARX, NARX and NARMAX Model Responses Compared with Actual Reactor Temperature T_r Data

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y - \hat{y}) \qquad (27)$$

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y - \hat{y})} \qquad (28)$$

Where, n is the number of samples, y is the actual outcome (Yadav et al., 2021) and $\hat{y}$ is the expected outcome (Yadav et al., 2021). Table 1 gives the MSE and RMSE error criterion values calculated to authenticate the best fit model.

The error criterion values clearly indicate that recursive least square based models have minimum error when compared with least mean square-based models.

Table 1: Error Criterion Values

Estimator	Model	Error	
		MSE	RMSE
lms	*ARX*	1.1789	1.0857
	NARX	21.586	4.646
	NARMAX	1.4938	1.222
rls	*ARX*	1.0316	1.0157
	NARX	1.0336	1.0167
	NARMAX	1.1581	1.0761

Conclusion

This work has addressed the best fit model for reactor temperature T_r and best estimation algorithm. the non-feedback test on differential equation of the batch reactor is conducted in simulation environment and the data is collected for the least mean square and recursive least square application, to identify ARX, NARX and NARX models. Then the performance of models is analyzed by the model responses and error criterion values. It is cleared that recursive least square based NARX model is best fit for reactor temperature T_r. the recursive lest square NARX model performs more precisely when compared with least mean square NARX model proposed in the literature. Even though the error criterion values of NARMAX model is low but the transient response is not smooth when compared with NARX model, thus this study proposed the recursive least square based NARX model for further work. In future nonlinear model-based controller NMBC is going to be developed for the polymerization batch reactor in that recursive least square based NARX model T_r will be used as refence model.

Appendix

Nomenclature

The following are the differential equation model parameters abbreviations (Yadav et al., 2021; Shettigar et al., 2021).

[I]	initiator concentration
[M]	monomer concentration
α, β	heat loss coefficents
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_r	reactor 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 differential equations parameter values are as follows (Yadav et al., 2021; Shettigar et al., 2021).

$A = 4.4*10^{16}$ s-1

$A_p = 2.833*10^9$ L0.75mol-0.75s-1

$E_d = 140.06*10^3$ J

$E_p = 7.0711*10^4$

R = 8.3145 J/ (mol K)

ε = 0.5

θ = 1.25

V = 0.5 L

$\Delta H_p = -82.2*10^3$ J/mol

$P_0 = 10.72035$

$\rho = 1000.05*10^3$/m3

n = 200 rpm=3.33rps

d = 0.05m

α = 1.0003W°C^(-β)

$\beta = 0.001845$

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

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