

Support Vector Regression Based Model Identification of a Batch Reactor Process: A Simulation Study

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Abstract

The present study emphasizes the use of Support Vector Regression-based model identification for acrylamide polymerization reaction in a batch reactor process with three kinds of SVR kernels. The real-time plant is identified by solving the differential equation models of the plant. The first model identification approach is done using Linear Kernel, the second model identification approach is done using Polynomial Kernel, and the third one is done using Radial Basis Function. In all three approaches, the cost function is defined for equal penalization of all errors. The study emphasizes machine learning-based model identification of the non-linear system.

Keywords: Support Vector Regression SVR, Reactor Temperature T_r , Jacket Temperature (T_j), Initiator Ammonium Persulphate Concentration I , Monomer Concentration (M), Output Y , Target T .

Introduction

The exothermic reactions are carried out in the batch reactor so that monomer-to-polymer conversion can be achieved. In that way, there will be n variables that are responsible for the product formation. In this manner, the batch process will be a very non-linear process, and here, the feed is not fed to the reactor continuously; rather, the feed compound is fed to the reactor in a particular time period. Here, the reactor temperature T_r and jacket temperature are the important parameters for the product formation, which leads us to conclude that regulating the reactor temperature through the manipulation of coolant flow rate can achieve the objective. Therefore, the solution to the problem consists of finding the best possible model that would help us to design the best control strategy (Arshad et al., 2021).

Simulation-based analysis for SVR-based model identification of a batch reactor is discussed in this work. From the literature review on Creation and verification of sophisticated nonlinear predictive control algorithms and data-driven pilot batch reactor modeling, get a complete white box differential equation model of a pilot plant batch reactor (Yadav et al., 2021). Open-loop test data are identified from the solution of the plant differential equation model. Recent studies on Hammerstein model identification of batches using neural networks reactors provide us with a complete picture of the development of a black box model using neural networks (Balakrishnan et al., 2023) (Aguado et al., 2009). ARX and NARX model identification has been performed in modeling a prototype batch reactor using data (Yadav et al., 2021).

A hybrid model involving both mechanistic and machine learning models to predict nitrous oxide (N_2O) provides us with the details of SVR implementation, feature selection, and preprocessing of data (Mehrani et al., 2022). Machine learning theories, concepts, and applications for engineers and system designers⁵ provides us with the basic concepts of machine learning, its types, and applications in real time. Big data approach to batch process monitoring⁶ taught us the use of support vector regression in fault detection (Ahmad Yasmin et al., 2021) (Zaidi, 2012) (Hossain et al., 2022).

Different kinds of kernels are available, but in this work, selected kernels are the linear kernel, the polynomial kernel, and the radial basis function kernel. The selection of these kernels is done through the literature provided by the past research, and the whole parameters of differential equations are obtained from the past literature (Shettigar et al., 2021) (Mehrani et al., 2022) (Onel et al., 2018).

Batch reactors find wide applications in the fields of polymerization processes and specialty chemicals production owing to their flexible operations and control over reaction time, composition, and temperature. However, due to the nonlinearity of reactor dynamics caused by complicated reaction kinetics, heat generation, varying concentrations of reactants, and interrelations between reactor and jacket temperatures, accurate modeling is necessary for temperature estimation, safety considerations, product quality enhancement, and further designing of advanced controllers. On the one hand, conventional models based on physicochemical principles are complicated, on the other hand – linear models are not always able to describe the behavior of nonlinear reactors properly. Thus, in this work Support Vector Regression-based identification of a batch reactor for acrylamide polymerization with use of open-loop simulation data acquired from nonlinear mass- and energy-balance equations will be investigated. Linear, second-order polynomial, and Radial Basis Function kernels will be comparatively studied after data preprocessing and feature selection based on correlations. Performance of the kernels will be evaluated according to mean absolute error, root mean square error, and coefficient of determination.

In all three cases, the SVR cost function will be mean square error minimization because for SVR, the goal is to have a minimum of ϵ , which is a function of error. Lower ϵ means better learning and fitting. In the first method, a linear function is considered despite the system being linear because it demonstrates the contradiction of linear kernels with respect to non-linear systems. In the second method, a polynomial function of order 2 is used to demonstrate how a non-linear function performs on non-linear systems, and finally, in the third method, a radial basis function is selected because it is a more powerful non-linear kernel than the former.

Batch Reactor

The complete arrangement of the batch polymerization reactor is shown in fig. 1 (Shettigar et al., 2021). The whole system is connected to the computer through the data acquisition card. The dimensions are, Inner diameter of the reactor = 101.6 mm, Outer diameter of the reactor = 197 mm, Inner height of the reactor = 169 mm, External height of the reactor = 183 mm, Length of the coolant coil = 1340 mm, Outer diameter of the coolant coil = 6.35 mm, Area of the batch reactor (A) = 0.06824193 m^2 , Heat transfer coefficient (U) = 500 $Wm^{-2} K^{-1}$, Heater wattage = 1500 W (maximum), Pressure range = 100 bar (maximum), Control valve (pneumatic air to close type 3-15 psi), Agitator 1200 rpm (maximum).

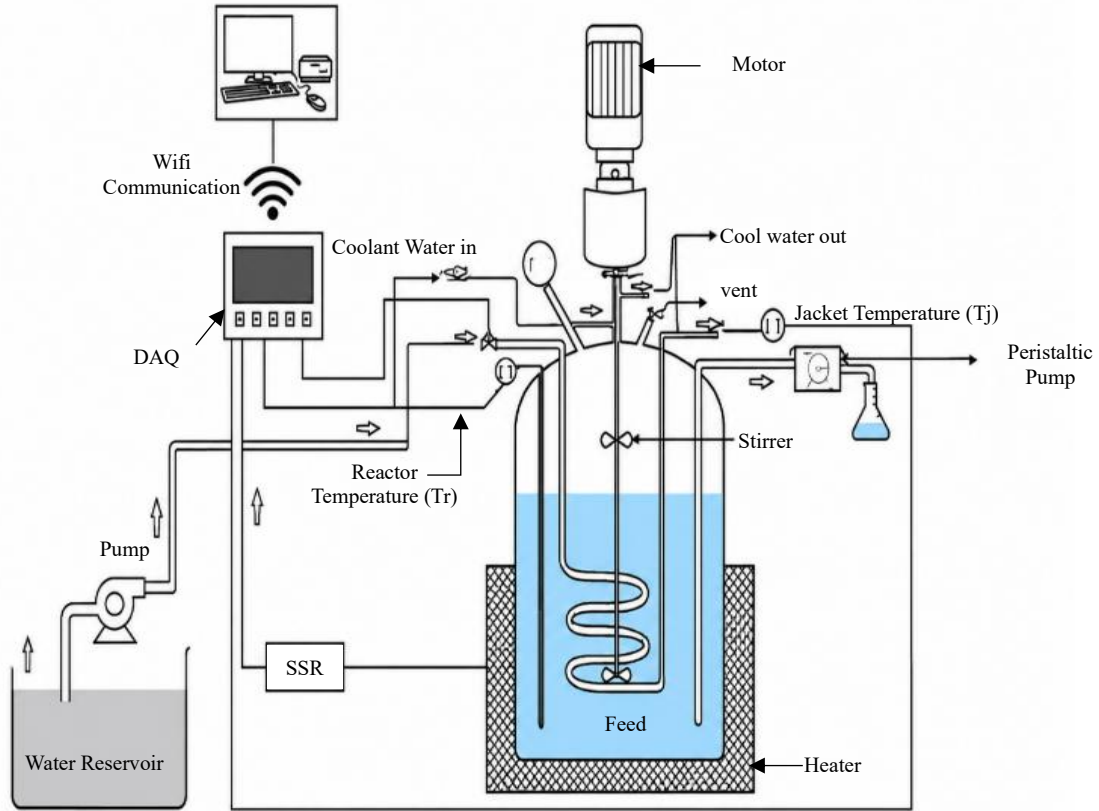


Fig. 1: Batch Polymerization Reactor

Mass Balance

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

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

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

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

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

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

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

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

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

Equations (1)– (9) are the representation of the nonlinear mechanistic model of the batch reactor using the principles of reaction rate chemistry along with the reactor and jacket heat balance equations. Open Loop Testing is performed using the following criteria: the initial reactor and jacket temperatures are taken as 55°C and 36.8°C, respectively; the flow rate of the coolant is kept constant at Coolant and ambient temperatures are regarded as being equal at 0 and 0.75 Lpm, or 0.1 kg/s (Shettigar et al., 2021). The parameters of the reaction mixture are 500 milliliters of 10% monomer, 5 milliliters of 0.009 mol/l, and $[Q_h F_c] = [60 \ 70]$ to achieve a steady state, followed by a step change to $[60 \ 50]$.

Open-loop simulation is performed in the MATLAB simulation environment, and the necessary data are obtained from the experiment. These data are used in training the SVR model with various kernels. The best fit algorithm will be used for developing nonlinear control systems in the future.

Support Vector Regression

Support Vector Machine is one kind of machine learning algorithm used for solving classification problems in the early time, but afterward, it was more often applied to solve regression problems (Jordan & Mitchell, 2015) (Aya et al., 2016).

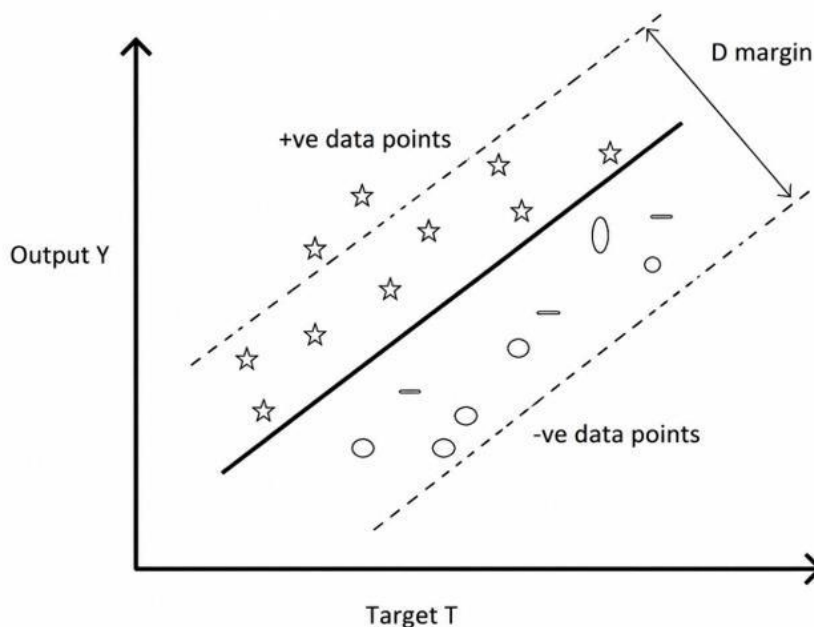


Fig. 2: SVR Hyperplane

SVR generates hyperplanes and two parallel hyperplanes that are nearer to one of the positive or negative data points shown in fig. 2. In SVR, the goal is to maximize the marginal distance for fitting the maximum data. The data points that are in the parallel hyperplanes are called support vectors. The flow chart involved in support vector regression is shown in fig. 3. SVR makes use of a kernel, which is used to convert the hyperplane from a low dimension to a high dimension, as the higher the dimension of the hyperplane, the greater the margin D.

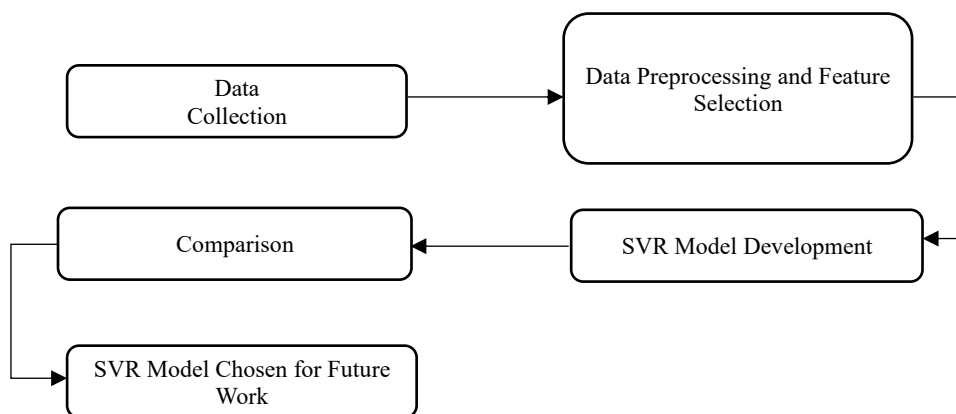


Fig. 3: SVR implementation Flow Chart

Data Preprocessing

Input for the training set is data from the open loop. Normalization or scaled value is between 0 and 1 range, presented in equation (10).

$$X_n = \frac{X_i - X_{min}}{X_{max} - X_{min}} \quad (10)$$

Where X_n is the normalized data; X_{max} and X_{min} are the maximum and minimum of the selected data, respectively; X_i is the value of the variables in the record.

Feature Selection

Pearson Correlation Coefficient (PCC): It is one of the techniques for feature selection (Halim et al., 2021). The value of PCC varies between +1 and -1 where +1 shows the positive correlation, -1 shows negative correlation, and 0 shows no correlation. It can be calculated using equation (11).

$$\sigma_{ij} = \frac{cov(f_i, f_j)}{\sqrt{var(f_i)var(f_j)}} \quad (11)$$

Where σ_{ij} is the correlation coefficient between the chosen feature f_j , cov , var , and every other feature covariance and variance.

SVR Based TR Prediction

Training data has a great impact on the prediction of the SVR8 model. Data that are not in the decision boundary will be ignored in order to avoid over-fitting. When predicting real numbers (an infinite number of choices) in SVR, it is quite troublesome; an error margin is used for the prediction (Mehrani et al., 2022). The nonlinear SVR function is shown in equation (12).

$$F(X) = \sum_{i=0}^M (\alpha_i - \alpha_i^*) K(X_i, X) + \delta \quad (12)$$

Where K is the transformation kernel with a dot product of the mapped vectors of the support vectors, M is the total number of training set instances, α_i , α_i^* are the LaGrange multipliers, and δ is some bias.

Linear Kernel

It is applied when data is linear or almost linear, but it can be used only for linear operations. Equation (13) represents the linear kernel,

$$K(X_i, X) = X_i^T \cdot X \quad (13)$$

Polynomial Kernel

It is a form of nonlinear kernel and is described in terms of the equation (14)

$$K(X_i, X) = \gamma (X_i^T \cdot X + C_0)^d \quad (14)$$

Where γ stands for the influence parameter and by default it is considered as 1 per feature, C_0 is the bias and it is always taken as 0 or 1, d is the order of the polynomial and here d is 2.

RBF Kernel

The RBF kernel is nonlinear kernel that can map data into nonlinear dimensions. It is represented using equation (15)

$$K(X_i, X) = \exp(-\gamma \text{norm}(x_i - X)^2) \quad (15)$$

Influence factor γ is set to 1 by default but can be selected depending on the system nonlinearity; lower γ makes borders fit better, higher γ influences localized data more.

Cost Function

Cost function is the optimization function that helps in making the prediction. In this case, cost function is based on the error function ε , weight vector W is the minimization function, lesser the ε more accurate is the model. It is denoted by equation (16).

$$\text{Minimize: } \frac{1}{2} \text{norm}(W)^2 + C \sum_{i=1}^n (\varepsilon_i + \varepsilon_i^*) \quad (16)$$

On condition,

$$\begin{cases} Y_i - W^T \phi(X_i) - b \leq \varepsilon + \varepsilon_i^* \\ W^T \phi(X_i) + b - Y_i \leq \varepsilon + \varepsilon_i^* \\ \varepsilon, \varepsilon_i^* \geq 0, \forall i \end{cases}$$

Values of parameters for SVR have been given in table 1.

Table 1: SVR Parameters

SVR	SVR-Linear	SVR-polynomial	SVR-RBF
ϵ	0.0010	0.0100	0.0010
C	1	10	100
γ	-	1	1
Bias term	0.8643	0.8643	0.8643
σ	-	-	10

Results

Performance Indices

In this study, the performance of the models has been assessed using goodness-of-fit R^2 and root mean square error and mean absolute error⁴, which are shown in equation (17), (18) and (19),

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}} \quad (17)$$

$$RMSE = \sqrt{\frac{SS_{res}}{n}} \quad (18)$$

$$MAE = \frac{1}{n} \sum_i (Y_i - f_i) \quad (19)$$

Where SS_{res} is sum of square of residuals, SS_{tot} is total sum of squares⁴. In table 1 have the values for the performance indices,

Table 2: Performance Indices

Performance indices	MAE	RMSE	R^2
SVR-Linear	2.5898	1.0589	-0.2389
SVR-Polynomial	0.3898	0.9452	-0.2237
SVR-RBF	0.0045	0.0123	0.998

Table 2, SVR with RBF kernel performs well for reactor temperature data; this is supported by the graphs as well. The reason behind this is that RBF kernel is capable of dealing with high nonlinearity, while polynomial kernel, which is also a nonlinear kernel, is appropriate for highly complicated data. Coming to the case of linear kernel, it should not be used in nonlinear data.

Model Response

Response of the models is presented in the below figures. The responses for Linear-SVR are presented in fig. 4 & fig. 5, Polynomial-SVR are presented in fig. 6 & fig. 7, and RBF-SVR are presented in fig. 8 & fig. 9.

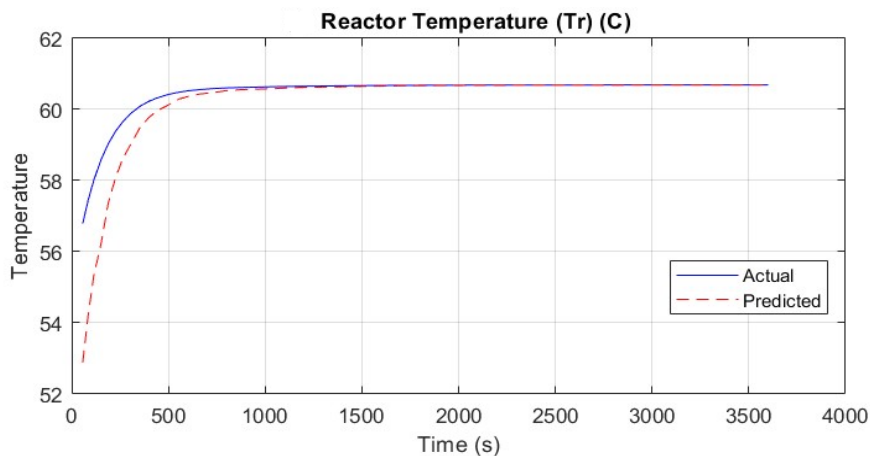


Fig. 4: SVR-Linear model of Batch Reactor

Fig. 4 represents the prediction response curve of the temperature using the Linear SVR model, which fails to provide accurate modeling of the nonlinear temperature behaviour in the batch reactor process.

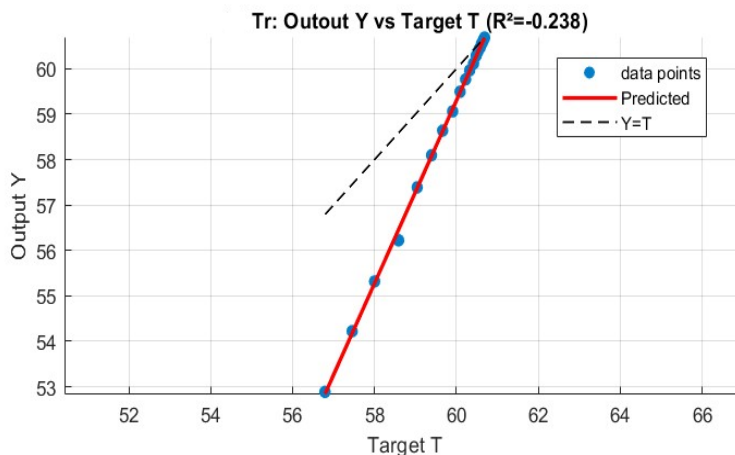


Fig. 5: Regression Fit of SVR-Linear of Batch Reactor

Fig. 5 illustrates the fitting performance of the Linear SVR model, which has low correlation between the actual and predicted reactor temperature values due to the nonlinear nature of the process.

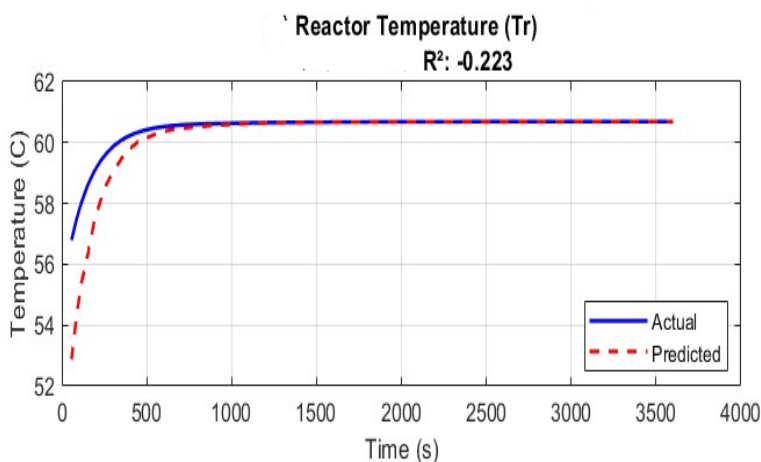


Fig. 6: SVR-Polynomial model of batch reactor

Fig. 6 illustrates the prediction response curve of the temperature of the batch reactor process using the Polynomial SVR model, which has better nonlinear modeling capability than the linear one but not very accurate.

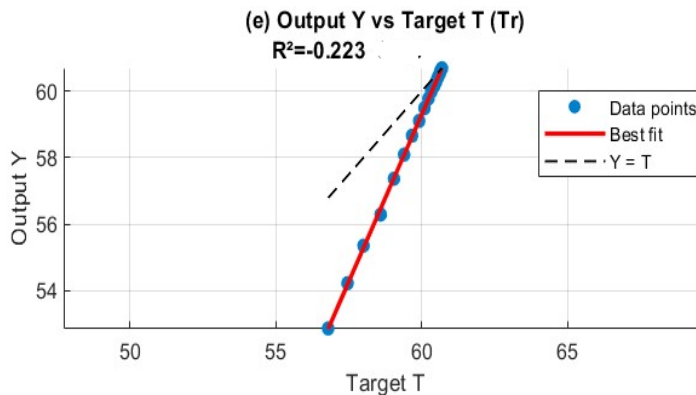


Fig. 7: Regression Fit of SVR-Polynomial Model of Batch Reactor

Fig. 7 demonstrates the regression relationship of the actual and predicted temperature values using the Polynomial SVR model, with moderate fitting performance for nonlinear processes.

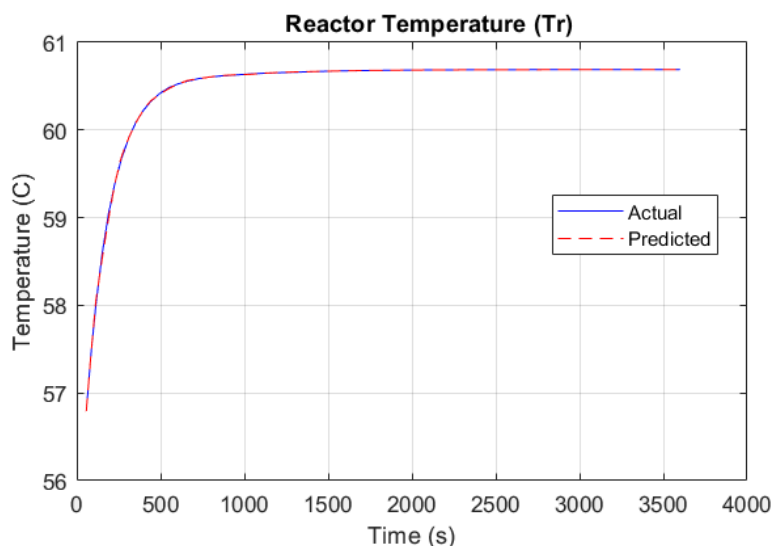


Fig. 8: SVR-RBF model of batch reactor

Fig. 8 represents the prediction response curve of the reactor temperature using the RBF-SVR model, with high capability of nonlinear dynamic behaviour modeling of the process.

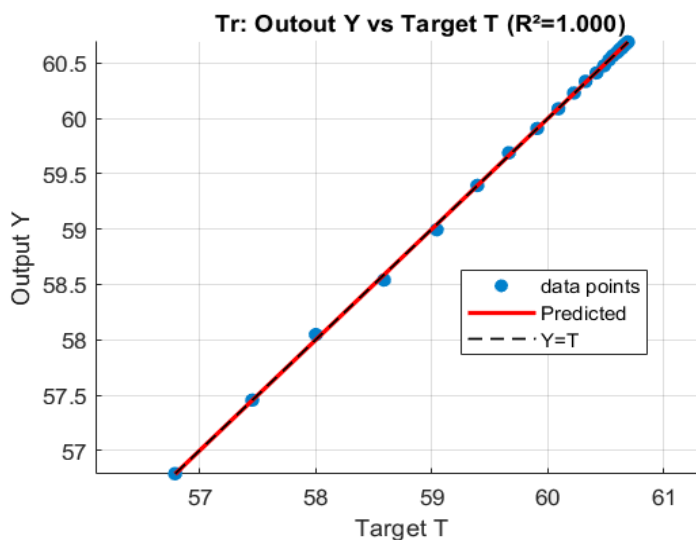


Fig. 9: Regression Fit of SVR-RBF Model of Batch Reactor

Fig. 9 shows the fitting performance of the RBF-SVR model with high agreement between predicted and actual reactor temperatures.

Conclusion

Three kinds of kernels are used in support vector regression for developing a model for batch reactor temperature. The SVR linear model is supposed to capture the reactor temperature; however, this is not happening, and similarly, the SVR polynomial model does not capture the temperature, despite having a polynomial kernel. The SVR RBF model gives a more accurate fit compared to the other two models. The SVR model will now be used in real-time processes, and results will be compared to the simulation results. After that, a non-linear model-based controller will be developed.

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Abbreviations

Non-Linear Model Parameters [1,2]

$$A = 4.4 \times 10^{16} \text{ s}^{-1}$$

$$A_p = 2.833 \times 10^9 \text{ L}^{0.75} \text{ mol}^{-0.75} \text{ s}^{-1}$$

$$E_d = 140.06 \times 10^3 \text{ J}$$

$$E_p = 7.0711 \times 10^4$$

$$R = 8.3145 \text{ J/(mol K)}$$

$$\epsilon = 0.5$$

$$\theta = 1.25$$

$$V = 0.5 \text{ L}$$

$$\Delta H_p = -82.2 \times 10^3 \text{ J/mol}$$

$$P_0 = 10.72035$$

$$\rho = 1000.05 \times 10^3 / \text{m}^3$$

$$n = 200 \text{ rpm} = 3.33 \text{ rps}$$

$$d = 0.05 \text{ m}$$

$$\alpha = 1.0003 \text{ W}^\circ \text{C}^{-\beta}$$

$$\beta = 0.001845$$

$$m_1 = 450 \text{ g}$$

$$m_2(\text{initial}) = 4.5 \times 10^{-5} \text{ mol}$$

$$m_3(\text{initial}) = 0.734 \text{ mol}$$

$$m_4(\text{initial}) = 0 \text{ mol}$$

$$m_5 = 220 \text{ g}$$

$$m_6 = 7200 \text{ g}$$

$$m_7 = 18 \text{ g}$$

$$m_8 = 240 \text{ g}$$

$$C_{p1} = 4.184 \text{ J/g}^\circ \text{C}$$

$$C_{p2} = 187 \text{ J/mol }^\circ \text{C}$$

$$C_{p3} = 110.58 \text{ J/mol }^\circ \text{C}$$

$$C_{p4} = 84.95 \text{ J/mol }^\circ \text{C}$$

$$C_{p5} = 0.49 \text{ J/g}^\circ \text{C}$$

$$C_{p6} = 0.49 \text{ J/g}^\circ \text{C}$$

$$C_{p7} = 4.184 \text{ J/g}^\circ \text{C}$$

$$C_{p8} = 0.49 \text{ J/g}^\circ \text{C}$$

$$T_{amb} = 27^\circ \text{C}$$

Nomenclature [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
Cp1	specific heat of the solvent
Cp2	specific heat of the initiator
Cp3	specific heat of the monomer
Cp4	specific heat of the polymer
Cp5	specific heat of the stirrer
Cp6	specific heat of the reactor wall
Cp7	specific heat of the coolant fluid
Cp8	specific heat of the cooling coil
Cpc	specific heat of the coolant
d	diameter of the stirrer blades
Ed	dissociation enthalpy
Ep	polymerization enthalpy
Fc	coolant flow rate
m1	mass of the solvent(water)
m2	number of moles of initiator
m3	number of moles of monomer
m4	number of moles of polymer
m5	mass of stirrer
m6	mass of reactor vessel
m7	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
Tc	coolant temperature
Tj	jacket temperature
Tr	reactor temperature
Tamb	ambient temperature
U	overall heat transfer coefficient
V	volume of the reaction mixture

Ad	dissociation constant
Ap	polymerization constant
ρ	density of the reaction mixture

References

- Shettigar J, P., Lochan, K., Jeppu, G., Palanki, S., & Indiran, T. (2021). Development and validation of advanced nonlinear predictive control algorithms for trajectory tracking in batch polymerization. *ACS omega*, 6(35), 22857-22865. <https://doi.org/10.1021/acsomega.1c03386>
- 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>
- 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>
- Jordan, M. I., & Mitchell, T. M. (2015). Machine learning: Trends, perspectives, and prospects. *Science*, 349(6245), 255-260. <https://doi.org/10.1126/science.aaa8415>
- Onel, M., Kieslich, C. A., Guzman, Y. A., Floudas, C. A., & Pistikopoulos, E. N. (2018). Big data approach to batch process monitoring: Simultaneous fault detection and diagnosis using nonlinear support vector machine-based feature selection. *Computers & chemical engineering*, 115, 46-63. <https://doi.org/10.1016/j.compchemeng.2018.03.025>
- Halim, S. Z., Quddus, N., & Pasman, H. (2021). Time-trend analysis of offshore fire incidents using nonhomogeneous poisson process through bayesian inference. *Process Safety and Environmental Protection*, 147, 421-429. <https://doi.org/10.1016/j.psep.2020.09.049>
- Ahmad Yasmin, N. S., Abdul Wahab, N., Ismail, F. S., Musa, M. A. J., Halim, M. H. A., & Anuar, A. N. (2021). Support vector regression modelling of an aerobic granular sludge in sequential batch reactor. *Membranes*, 11(8), 554. <https://doi.org/10.3390/membranes11080554>
- Arshad, U., Taqvi, S. A. A., Buang, A., & Awad, A. (2021). SVM, ANN, and PSF modelling approaches for prediction of iron dust minimum ignition temperature (MIT) based on the synergistic effect of dispersion pressure and concentration. *Process Safety and Environmental Protection*, 152, 375-390. <https://doi.org/10.1016/j.psep.2021.06.001>
- Zaidi, S. (2012). Development of support vector regression (SVR)-based model for prediction of circulation rate in a vertical tube thermosiphon reboiler. *Chemical engineering science*, 69(1), 514-521. <https://doi.org/10.1016/j.ces.2011.11.005>
- Aguado, D., Ribes, J., Montoya, T., Ferrer, J., & Seco, A. (2009). A methodology for sequencing batch reactor identification with artificial neural networks: A case study. *Computers & Chemical Engineering*, 33(2), 465-472. <https://doi.org/10.1016/j.compchemeng.2008.10.018>
- Hossain, S. S., Ayodele, B. V., Ali, S. S., Cheng, C. K., & Mustapa, S. I. (2022). Comparative analysis of support vector machine regression and Gaussian process regression in modeling hydrogen production from waste effluent. *Sustainability*, 14(12), 7245. <https://doi.org/10.3390/su14127245>
- Aya, S. A., Acar, T. O., & Tufekci, N. (2016). Modeling of membrane fouling in a submerged membrane reactor using support vector regression. *Desalination and Water Treatment*, 57(51), 24132-24145. <https://doi.org/10.1080/19443994.2016.1140080>