

Design of Soft Computing Based Nonlinear Model Predictive Controller for the CSTR Process

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Abstract: In this brief, a soft computing Least Square Support Vector Machines (LSSVM) based Nonlinear Model Predictive Controller (NMPC) is proposed for the Continuous Stirred Tank Reactor (CSTR) process. Model predictive control (MPC) is a digital control scheme that works based on the prediction and control horizon. The Linear MPC (LMPC) based on analytical linearization uses linear models to predict the future behavior of the process and these linear models are not sufficient to describe about the performance of nonlinear dynamic systems. The Nonlinear MPC (NMPC) characterized by nonlinear models can describe the dynamic behavior of the nonlinear process. NMPC provides the same competences for constraint supervision as its linear equivalent. In this work, NMPC based on LSSVM models has been proposed to describe the dynamic behavior of the nonlinear process and the performance is measured through Integral Squared Error (ISE) and Integral Absolute Error (IAE). The performance of the proposed scheme is compared with Neural Network based MPC to show effectiveness.

Key words: CSTR • Integral Squared Error • LSSVM • Neural Networks • Model predictive control

INTRODUCTION

In process industries, most of the processes such as batch reactor, heat exchanger, distillation column, CSTR, etc. exhibits highly nonlinear behavior in nature. The linear MPC [1] derived based on local linear state is not sufficient to handle the process variations. The Nonlinear MPC (NMPC) [2,3] characterized by nonlinear models can describe the dynamic behavior of the nonlinear process. In this work, NMPC [4, 5] based on LSSVM [6] model has been proposed to describe the dynamic behavior of the nonlinear process.

The local linear models are derived around the steady state and linear MPC (LMPC) is designed from the analytical linearization model [7-9]. The linear models are combined by Takagi-Surgeon (T-S) techniques to form the Analytical linearization Nonlinear MPC (A-NMPC) [9]. The A-NMPC selects the controller based on the present operating region through the switching scheme. Both LMPC and A-NMPC is works based on local linear model [10], but real time CSTR process operates over the wide region. Therefore, the soft computing techniques viz. Neural Network, Fuzzy, Support Vector Machines (SVM),

etc. can be used to predict the entire plant model. The Neural Network based NMPC (NN-NMPC) [11-13] involves huge training requirement, poor generalization ability and over-fitting issues.

The SVM [12] introduced by Vapnik (1998) overcomes the generalization and over-fitting issues of neural network model. SVM has strong generalization ability for the nonlinear systems, but requires large number of kernels to find the optimal solution. The LSSVM introduced by Suykens based on SVM uses an equality constraint which is used to eliminate the quadratic programming problem solving and reduce the run time. LSSVM finds the solution by solving linear equations and increases the performance of the model [6, 7]. In LSSVM, the mapping between input space and the feature higher dimensional space can be implemented through the kernel function. The different kernel functions such as linear, Multi-Layer perceptron and Radial Basis Function are used to find the mapping between input and output [2, 7]. In this paper, LSSVM based NMPC is presented to the CSTR process and the results demonstrates the performance of the proposed scheme when compared to A-NMPC and NN-NMPC [1, 3].

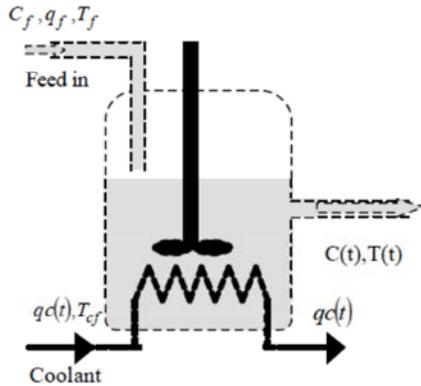


Fig. 1: CSTR Process

This paper comprises of six sections starting with the introduction as the section.1. Section.2 explains the CSTR process description. Section.3 demonstrates A-NMPC and NN-NMPC design. Section.4 discusses about NN based NMPC. Section.5 demonstrates the performance of proposed LSSVM based NMPC scheme for the CSTR process and the simulation studies are also given. The detailed conclusion of work done is given in section [14].

CSTR Process Description: The Schematic diagram of the CSTR used in this work is shown in Figure 1 [9, 10]. The reactant 'A' is feed to the reactor with a volumetric flow rate Q_f , a molar concentration (or composition) C_f and a temperature T_f . The components inside the reactor are well mixed with a motorized stirrer. Both the reactant A and product B are withdrawn continuously from the reactor with a flow rate, a concentration C and a temperature T . To remove the exothermic heat that is generated due to the chemical reaction, coolant is circulated outer side of the reactor. A inlet coolant stream with a volumetric flow rate q_c and an inlet temperature T_{cf} continuously take out the heat to maintain the desired reaction temperature.

The objective of the controller design here is to keep the concentration $C(t)$ and temperature (T) of the product into desired range by adjusting the inlet coolant flow rate $q_c(t)$. The nominal initial parameter settings of the process considered in this study are given in Table 1 [9].

In order to identify the model of CSTR, the mass, energy and component balance equation must be properly described. The derivation of these balance equations needs a background study about the parameters involved in the CSTR and its chemical reactions during the operation. From the mass, energy and component balance

Table 1: CSTR Parameters

Process parameter	Initial operating condition
Inlet feed flow rate (q_f)	100 l/min
Inlet feed temperature (T_f)	350 K
Inlet coolant temperature (T_{cf})	350 K
Inlet concentration (C_f)	1 mol/l
Volume of the tank (V)	100 l
Activation energy (E/R)	1×10^4 K
Reaction rate constant (K_0)	$7.2 \times 10^{10} \text{ min}^{-1}$
Heat reaction	$-2 \times 10^5 \text{ cal/mol}$
Liquid density (ρ)	$1 \times 10^3 \text{ g/l}$

equations, the model describing the rate of change of composition (concentration) and temperature in the system is then given by Equation. 1) and Equation (2).

$$\frac{dT}{dt} = \frac{q_f}{V}(T_f - T(t)) + K_1 C(t) \exp\left(-\frac{E}{RT(t)}\right) + K_2 q_c(t) \left[1 - \exp\left(-\frac{K_3}{q_c(t)}\right)\right] (T_{cf} - T(t)) \quad (1)$$

$$\frac{dC}{dt} = \frac{q_f}{V}(C_f - C(t)) - K_0 C(t) \exp\left(-\frac{E}{RT(t)}\right) \quad (2)$$

The open-loop responses of CSTR temperature and concentration when the coolant flow rate $q_c(t)$ varies from 85 l/min to 110 l/min are given in Figure 2 and Figure 3. From the responses, it is observed that the parameters are varying from over-damped to underdamped which shows non-linear dynamical behavior of the process [10].

A linear state space model will be derived around the steady state operating point. From the initial parameters and state space model, the following initial operating regions and corresponding Eigen values are given in Table 2 are derived.

Analytical Linearization Based LMPC and NMPC: The identification of state variables in nonlinear CSTR system is carried out by taking coolant flow rate (q_c) as the premise variable and the local model parameters are determined by linearizing the nonlinear differential equations based on analytical linearization [4, 8]. The linear model derived at nominal input values of coolant flow rate (q_c), Feed Temperature (T_f), Feed flow (q_f), feed concentration (C_f) initial concentration C_0 and Initial Temperature T_0 (state vectors- C_0, T_0) with the sampling time of 0.83 seconds.

Linear Model Predictive Controller: The linearized mathematical which is derived using analytical linearization is used to construct MPC.

Table 2: CSTR Stable operating regions

Operating region	Eigen values	Stability
$C_A = 0.0795, T = 443.4566, q_c = 97$	$\lambda_1 = -1.0; \lambda_2 = 1.5803$	Saddle point
$C_A = 0.0885, T = 441.1475, q_c = 100$	$\lambda_1 = -2.3899; \lambda_2 = -1.0$	Stable
$C_A = 0.0989, T = 438.7763, q_c = 103$	$\lambda_1 = -7.7837; \lambda_2 = -1.0$	Stable
$C_A = 0.1110, T = 436.3091, q_c = 106$	$\lambda_1 = -24.9584; \lambda_2 = -1.0$	Stable
$C_A = 0.1254, T = 433.6921, q_c = 109$	$\lambda_1 = -59.8325; \lambda_2 = -1.0$	Stable

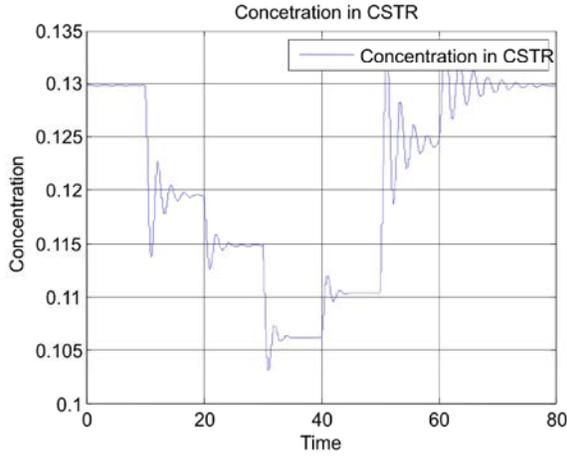


Fig. 2: CSTR Concentration - open loop response

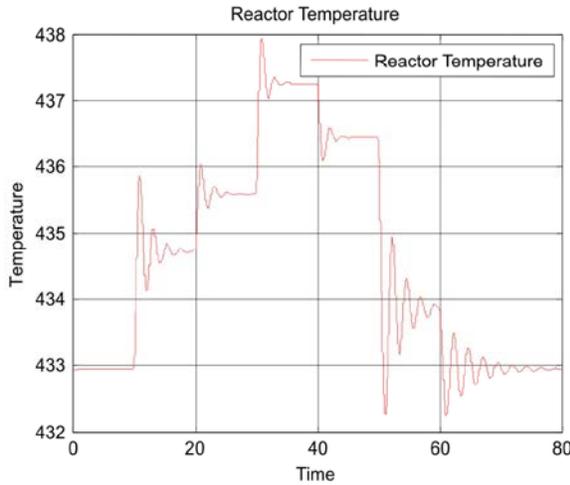


Fig. 3: CSTR Temperature - open loop response

In general, the state space is expressed as in Equation (3).

$$\dot{X} = Ax + Bu \quad Y = Cx + Du \quad (3)$$

The input, output and state of the system is expressed as deviation variable form given in Equation (4)

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} C_A - C_{As} \\ T - T_s \end{bmatrix} = \begin{bmatrix} 0.0885 \\ 350 \end{bmatrix}$$

$$y = T - T_s = 350$$

$$u = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} T_j - T_{js} \\ T_f - T_{fs} \\ C_{Af} - C_{Afs} \\ F - F_s \end{bmatrix} = \begin{bmatrix} 350 \\ 100 \\ 1 \\ 102.9 \end{bmatrix} \quad (4)$$

Where T_j is the jacket temperature and T_b, C_{Ab}, F are inputs.

The jacobian matrix is used to derive the state space of CSTR and the values A,B,C and D matrices are given in Equation (5).

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} -\frac{q}{V} - K_0 \exp\left(\frac{-E}{RT}\right) & -C_A K_0 \exp\left(\frac{-E}{RT}\right) \left(\frac{E}{TT}\right) \\ \frac{-\Delta H}{\rho C_P} K_0 \exp\left(\frac{-E}{RT}\right) & -\frac{F}{V} - \frac{UA}{V\rho C_P} + \frac{(-\Delta H)}{\rho C_P} C_{As} K_s^1 \end{bmatrix}$$

$$A = \begin{bmatrix} 8.5000 & 2.5938e+003 \\ -0.1000 & -14 \end{bmatrix}$$

$$B = \begin{bmatrix} b_{11} \\ b_{12} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial u_1} \\ \frac{\partial f_2}{\partial u_1} \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{UA}{V\rho C_P} \end{bmatrix} = \begin{bmatrix} -0.9346 \\ 0.0092 \end{bmatrix}$$

The output matrix is

$$c = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad d = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (5)$$

The LMPC servo response for the identified linearized model at input $u=[350 \ 1 \ 100 \ 100]$ with prediction horizon=8 and control horizon=2 is given in Figure 4. The linear model developed for particular region gives

Table 3: ISE and IAE values of the LMPC

Performance measure	Operating Region	Sampling instants				
		0-50	50-100	150-200	200-250	250-300
IAE	Linear region $u = [102.9 \ 350 \ 100 \ 1]$	0.5850	0.0208	0.0027	0.0021	0.0021
	Shifted region $u = [100 \ 350 \ 100 \ 1]$	0.9216	0.2524	0.2643	0.2569	0.2497
ISE	Linear region	0.0148	1.6206e-005	1.4811e-007	8.8530e-008	8.3835e-008
	Shifted region	0.0244	1.3e-003	1.4e-003	1.3e-003	1.2e-003

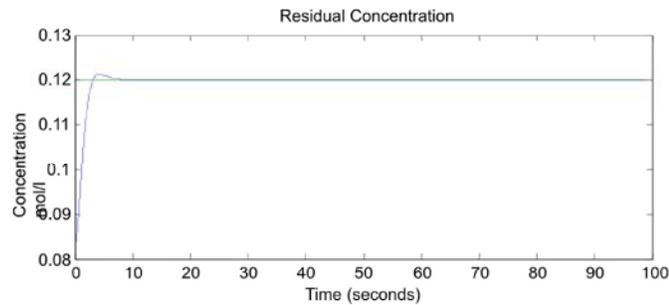


Fig. 3: Servo response of LMPC for input $u=[350 \ 1 \ 100 \ 100]$

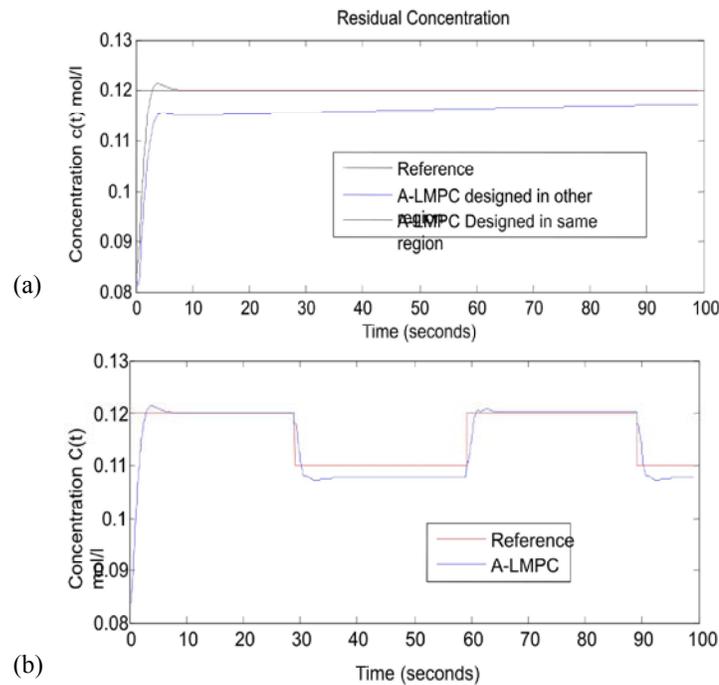


Fig. 5: Servo response comparison of LMPC

poor servo tracking performance in other region. For input $u= [350 \ 1 \ 100 \ 102.9]$, the servo response of the LMPC is given in Figure 5.a & b. From the response, it is observed that the prediction and control horizons doesn't have appreciable effects when input changes [Jp *et al*].

The performance of the LMPC for the identified linear region and for the shifted region is explained through the ISE and IAE values given in Table 3.

From the results, it is clear that model of the process is the key factor in the performance. LMPC provides

Table 4: Servo response ISE & IAE values NMPC

Performance measure	Controller	Sampling instants				
		300-350	350-400	400-450	450-500	500-550
ISE	A-LMPC	4.2253e-006	6.2311e-004	3.1165e-004	2.8137e-004	2.7934e-004
	A-NMPC	7.4586e-008	7.9326e-004	3.8119e-006	8.9725e-007	6.6120e-006
IAE	A-LMPC	0.0040	0.1508	0.1247	0.1186	0.1182
	A-NMPC	0.0020	0.1134	0.0128	0.0067	0.0182

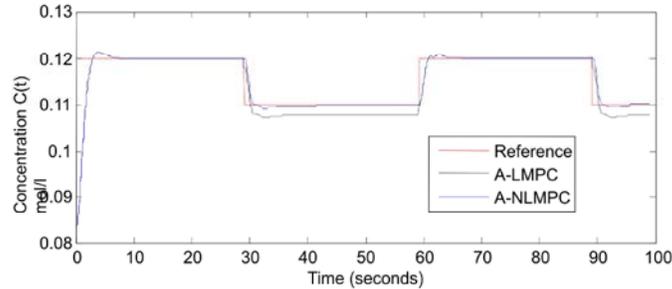


Fig. 6: Servo response of the NMPC scheme

better performance for the identified model; therefore it is not suitable for the nonlinear CSTR because it has varying operating condition

Analytical Linearization Based Nonlinear Model Predictive Controller (A-NMPC): The NMPC is formulated by combining different operating region linear MPC controllers and switching the control action accordingly to the current state of the plant. When the operating condition varies the switching scheme selects the appropriate controller and this adaptive control scheme enables the controller to provide improved performance than the LMPC scheme [8, 9].

The design of local model is done through the linearization of CSTR around the stable operating points and prediction is done from the local model. Therefore NMPC provides better performance in shifted operating regions. In NMPC, predictive controller is designed for each identified regions and respective controller is selected by simple switching scheme. If control coolant flow rate is below 50.438 l/min then the local model 5 is selected by the controller and if control action lies in the range of $50.438 < q_c < 68.78$ then the 4th local model is selected. The servo response of the NMPC is given in Figure 6.

The adaptive NMPC offers better performance than the LMPC because of the switching scheme. The performance measures given in Table 4 clearly show the effectiveness of NMPC than its counterparts under varying operating conditions.

From the results, it is find that both LMPC and NMPC based on local linear models only suitable for the identified regions around the process steady state. But in real time CSTR operates over wide operating range, therefore above discussed schemes are not suitable for the complex nonlinear systems. The performance can be improved only through the complete plant nonlinear model identification. The next section presents the soft computing techniques viz. Neural Network and Support Vector Machines based nonlinear model identification used in NMPC.

Neural Network Based NMPC: The neural network based MPC (NN-MPC) design involves the design of NN model which is used to predict future plant performance [13, 14]. The control action which minimizes the cost function is then calculated based on the prediction and then applied to the plant. The first step in MPC design is to determine the neural network that is trained to mimic the plant behavior (system identification) and then identification of the plant model which is derived by the neural network which is used by the controller to predict future performance.

The neural network with single hidden layer identify the plant feed forward model which is used to find the future trend of the process by predictions. The training is carried out using the learning algorithm that aims to minimize the error between the prediction and actual value. The training data generated using the classic experimental approach. The random input coolant flow

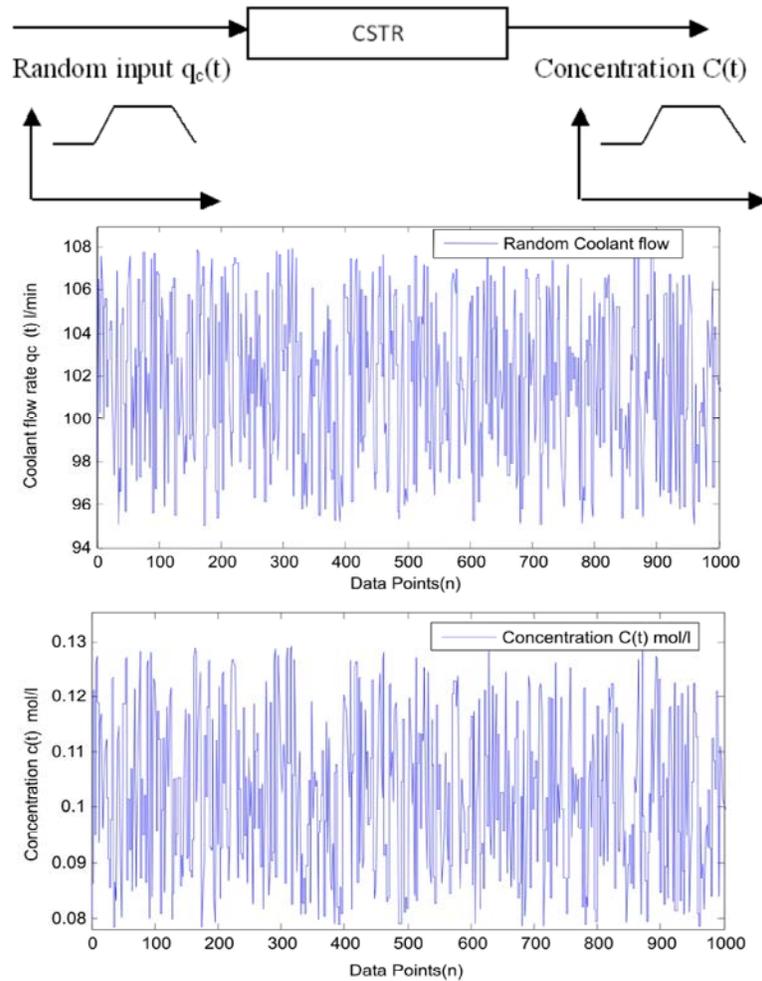


Fig. 7: Training data set of NN Model identification

rate profile is generated and the concentration output is taken as shown in Figure 7. The coolant flow rate is imposed to bound constraints from 95 to 108.

The data set of input and corresponding output is collected as given in Equation (6).

$$D^N = \{[u(t), y(t)], t=1, 2, 3, \dots, N\} \quad (6)$$

The number of neurons in the hidden layer is decided randomly. In this work, the number neurons assigned to 1500 and due to large number of neurons the NN is able to catch the forward dynamics appreciably. The prediction capability of trained the neural network is shown in Figure 8.

The performance measures of the NN-MPC and the comparison results are given in Table 5 and the results show that the NN based MPC outperforms than LMPC scheme.

From results, it is concluded that the neural network based NMPC works well in shifted operating regions than the analytical NMPC (A-NMPC).

LSSVM Based NMPC: The LSSVM based on SVM [3, 12] is presented by Suykens to eliminate the complex quadratic programming solving procedure. The identified LSSVM model uses the following function shown in Equation.(7) to approximate the unknown variable.

$$y(x) = w^T \phi(x) + b \quad (7)$$

Where $\phi(x)$ is a nonlinear mapping from the input space 'x' to a higher dimensional feature space, 'w' is the weight vector and 'b' is the bias. In LSSVM, the optimization function can be obtained by using the squared loss function and equality constraints, which give the optimization, function as shown in Equation (8).

Table 5: NN-MPC ISE & IAE performance comparison

Performance measure	Controller type	Sampling instants				
		300-350	350-400	400-450	450-500	500-550
ISE	A-LMPC	4.2253e-006	6.2311e-004	3.1165e-004	2.8137e-004	2.7934e-004
	A-NLMPC	7.4586e-008	7.9326e-004	3.8119e-006	8.9725e-007	6.6120e-006
	NN-NLMPC	4.2242e-006	6.2726e-004	3.1922e-004	2.8704e-004	2.8495e-004
IAE	A-LMPC	0.0040	0.1508	0.1247	0.1186	0.1182
	A-NLMPC	0.0020	0.1134	0.0128	0.0067	0.0182
	NN-NLMPC	0.0019	0.1133	0.0133	0.0065	0.0173

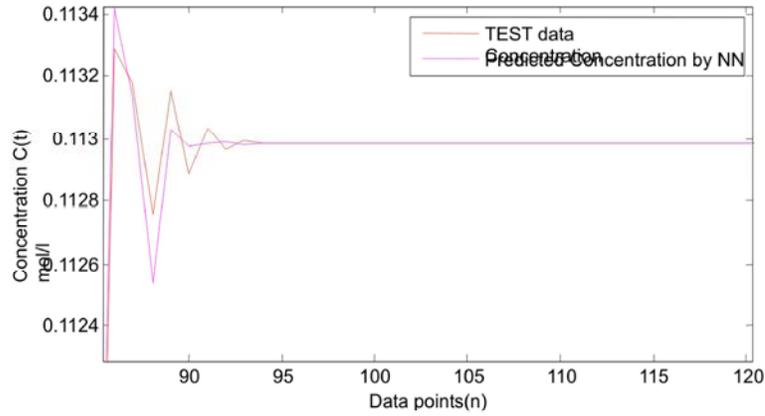


Fig. 8: Prediction performance of the NN-MPC scheme

$$\min J = \frac{1}{2} w^T w + C \frac{1}{2} \sum_{i=1}^N e_i^2 \quad (8)$$

Subject to the equality constraints

$$y(i+1) = w^T \varphi(x_i) + b + e_i \quad (9)$$

$i=1,2,\dots,n$

Where, e_k , the training error and C is the regularization parameter. Based on objective function and constraint condition, lagrangian function is constructed to solve the optimization problem and it is expressed in Equation (10).

$$y_z(k+1) = \sum_{i=1}^l \alpha_i K(x_i, x_j) + b \quad (10)$$

$$b = y(i+1) - \sum_{i,j=1}^n \alpha_i K(x_i, x_j)$$

Where α_i and b are the Lagrange multipliers which estimated based on the N training data set. Optimal condition of the Equation. (10) can be obtained through the solution of partial derivatives of L ($w, b, e; \alpha$) in Equation. (11) with respect to $w, b, e; \alpha$, i.e

$$\frac{\partial L}{\partial w} = 0 \Rightarrow w = \sum_{i=1}^N \alpha_i \phi(x_i) = \sum_{k=1}^N C e_{ki} \phi(x_i) \quad (11)$$

Substituting e_i and w with α_i and b , we can get LSSVM model as shown in Equation.(12) for the nonlinear process.

$$y_i = \sum_{i=1}^N \alpha_i K(x, x_i) + b \quad (12)$$

Where α_i and b are the solutions to the linear system and $K(x, x_i)$ is the kernel function satisfying the mercer condition, i.e. represents the mapping of input space x with high dimensional feature space. Based on the mercer condition one takes a kernel,

$$k(x, x_i) = \begin{cases} x_i^T x & \text{Linear} \\ (x_i^T x + 1)^p & \text{Polynomial, } p \in N \\ \exp\left[-\frac{C \|x - x_i\|^2}{2\sigma^2}\right] & \text{RBF} \end{cases} \quad (12)$$

Where ' σ ' is the kernel width parameter

The prediction performance of the LSSVM is shown in Figure 9 and the performances are listed in Table 6.

Table 6: ISE & IAE values of LSSVM-MPC

Performance measure	Controller type	Sampling instants				
		0-50	50-100	100-150	150-200	200-250
	NN-NLMPC	0.0148	1.6206e-005	1.4811e-007	8.8530e-008	8.3835e-008
	LSSVM-NMPC	0.0134	1.1731e-006	1.4811e-007	8.8530e-008	8.3835e-008
	NN-NLMPC	0.5760	0.00614	0.00279	0.00214	0.00217
	LSSVM-NMPC	0.5396	0.00598	0.00274	0.00213	0.00204

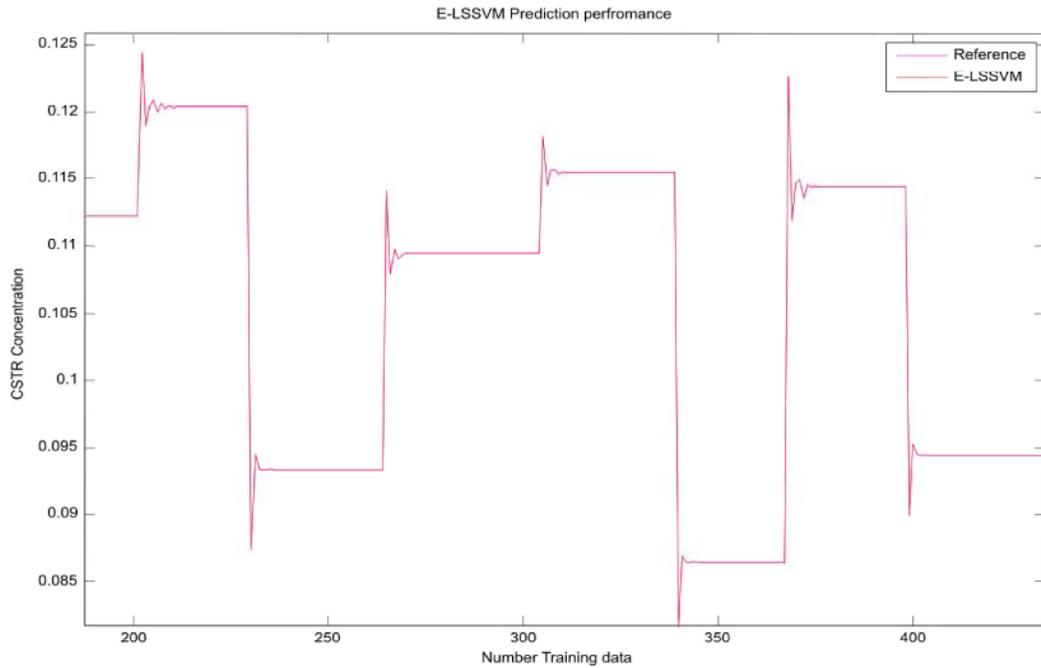


Fig. 9: Prediction performance of LSSVM-MPC

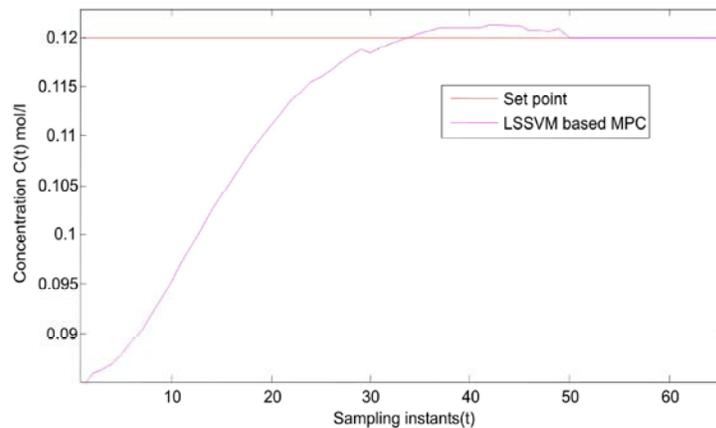


Fig. 10: Servo response of LSSVM - NMPC

The closed loop tracking servo performance of the LSSVM-NMPC is given in Figure 10 (a) & (b). From the results and ISE & IAE values, it is observed that the proposed LSSVM based approach outperforms than other methods.

CONCLUSION

The LSSVM based MPC provides better prediction performance and good generalization ability. In this paper, the LSSVM based NMPC controller is presented for the

CSTR process to get improved stability and closed loop tracking performance. Further, the performance of the LSSVM based NMPC is compared with other approaches. From the results, it can be concluded that the proposed NMPC helps to get better prediction needed for good servo and regulatory action. Hence the proposed NMPC can be considered as an alternative to conventional predictive controller. The effectiveness of the proposed scheme is proven through the closed loop performance and prediction performance of the CSTR process and the results are compared with its counter-part. The proposed method provides the better prediction with high accuracy and improves the generalization ability.

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