

Optimal Control of CSTR

Kalpesh Pathak, Anil Markana and Nishant Parikh

Abstract—Nonlinear Model Predictive Control (MPC) of Continuous Stirred Tank Reactor (CSTR) has been demonstrated in this work. Optimal state estimation has been done using Extended Kalman Filter (EKF). Second order mathematical model for CSTR has been developed and further used for dynamic simulations. It is found that optimal control of temperature inside the CSTR is achieved better with the help of MPC strategy compared to conventional control strategies. It is seen that setpoint tracking performance using this optimal control strategy is satisfactory achieved.

Index Terms—Model Predictive Control, Extended Kalman Filter, controller effort

I. INTRODUCTION

Chemical reactors together with mass transfer processes constitute an important part of chemical processes. From a control point of view, reactors belong to the most difficult nonlinear processes. We describe here CSTR as second order process where the aim is to control the temperature of product inside CSTR by manipulating the inlet steam temperature. Exothermic reactors are very interesting systems because of their potential safety problems and the possibility of exotic behavior such as multiple steady states. Furthermore, operation of chemical reactors is corrupted by many different uncertainties. Some of them arise from varying or not exactly known parameters like chemical kinetics or reaction activity. Operating points also change in this process. Various types of perturbations also affect chemical reactors. All these uncertainties can cause poor performance or even instability of closed-loop control systems. In this paper we concentrate on a CSTR as a highly nonlinear system. In the jacketed chemical reactor (CSTR) shown in Figure 1, a second-order exothermic reaction takes place, in which component A react irreversibly and at specific reaction rate to form a product. The reaction rate constant follows the Arrhenius equation. According to this equation, the effect of temperature, on the specific reaction rate is usually exponential. This exponential temperature dependence represents one of the most severe nonlinearities in chemical engineering systems.[7].

Patwardhan S.C. et. al.[5] used a discrete quadratic perturbation model for approximating nonlinear plant dynamics in the neighborhood of the operating point by simulating a benchmark CSTR system. Simulation with MPC with State Estimation and Adaptation Mechanism[7] for a CSTR has

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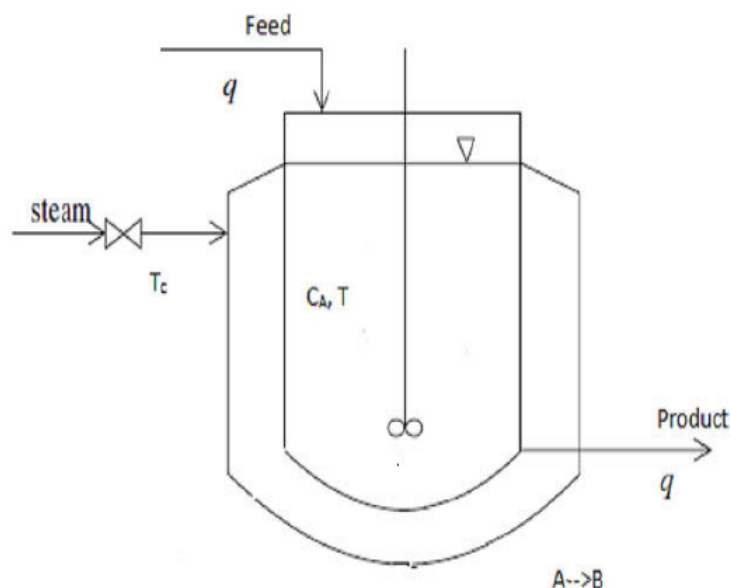


Fig. 1. Continuous Stirred Tank Reactor

been performed for normal operating conditions and with disturbances also. Past work includes classical control, Artificial Intelligence(AI), Neural Network(NN) and Fuzzy logic based control algorithm for CSTR.

Optimal control strategies like MPC and Linear Quadratic Gaussian (LQG) Control are effective here. MPC refers to a class of algorithms that compute a sequence of manipulated variable adjustments in order to optimize the future behavior of a plant. Adaptation of linear models with occurrence of new conditions according to variety of operating points in nonlinear systems is a solution for extending linear methods in design of controllers for nonlinear systems. Nonlinear MPC to control temperature inside CSTR has been presented here. Optimal state estimation has been done using Extended Kalman Filter (EKF). Second order mathematical model for CSTR has been developed and further used for dynamic simulations. Satisfactory set point tracking performance shows that optimal control of temperature inside the CSTR is achieved better with the help of MPC strategy compared to conventional control strategies.

II. MATHEMATICAL MODEL

In this section the mathematical model for the CSTR is derived. The process input and output are temperature of the steam and temperature of the product respectively.

Overall reactor material balance

The overall reactor material balance equation is.

$$\frac{d}{dt}v\rho = F_{in}\rho_{in} - F_{out}\rho \quad (1)$$

Where,

v : constant liquid reactor volume

ρ : density of reactor fluid

ρ_{in} : density of inlet stream

F_{in} : Flow rate of inlet stream

F_{out} : Flow rate of outlet stream

Assuming Constant density ($\rho_{in} = \rho$) and volume, it is easy to show that $F_{in} = F_{out} = F$.

Balance on component A

here we consider the simple reaction $A \rightarrow B$. The balance on component A is

$$v\frac{d}{dt}C_A = FC_{Af} - FC_A - Vr_A \quad (2)$$

Where,

C_A :Concentration of component A in the reactor

r_A :Rate of reaction per unit volume

The Arrhenius expression is normally used for the rate of reaction. A first-order reaction results in the following

$$r_A = k_0 \exp\left(\frac{-E_a}{RT}\right)C_A \quad (3)$$

Where,

k_0 :Frequency factor

E_a :Activation energy

R : Ideal gas constant

T :Reactor temperature on an absolute scale(Rankine or Kelvin)

Reactor energy balance

The reactor energy balance assuming constant volume, heat capacity (C_p) and density, and neglecting changes in the kinetic and potential energy is,

$$v\rho C_p \frac{d}{dt}T = F\rho C_p(T_f - T) + (-\Delta H) * Vr_A - U_A(T - T_j) \quad (4)$$

where,

$(-\Delta H)$: heat of reaction

U : Heat transfer coefficient

A : Heat transfer area

T_f :Feed temperature

T_j :Jacket temperature

State variable form of the equations

$$\frac{d}{dt}C_A = f_1(C_A, T) = \frac{F}{v}(C_{Af} - C_A) - k_0 \exp\left(\frac{-E_a}{RT}\right)C_A \quad (5)$$

$$\frac{d}{dt}T = f_2(C_A, T) = \frac{F}{v}(T_f - T) + \frac{(-\Delta H)}{\rho C_p} * k_0 \exp\left(\frac{-E_a}{RT}\right)C_A - \frac{U_A}{v\rho C_p}(T - T_j) \quad (6)$$

Taking state variable $x_1 = C_A$ and $x_2 = T$ above model can be written as nonlinear state variable form

$$\frac{d}{dt}x(t) = f(x, u) \quad (7)$$

where,

$x(t)$: state vector

$u(t)$: Input vector

The nonlinear dynamical Eqns for CSTR given by Eqn 5 & Eqn. 6, considering parameters and constants listed in Table I can be written as,

$$\frac{d}{dt}x_1 = D_a(1 - x_1) - \exp\left(\frac{x_2}{1 + \frac{x_2}{\gamma}}\right) - x_1 \quad (8)$$

$$\frac{d}{dt}x_2 = -x_2 + B(D_a(1 - x_1) - \exp\left(\frac{x_2}{1 + \frac{x_2}{\gamma}}\right)) + \beta(u - x_2) \quad (9)$$

The parameter values of the laboratory process are given in Table I

Parameters	Values
β	3
γ	40
B	22 DMA
Da	0.082 DMA
u	-2.5 DMA

TABLE I
PARAMETER VALUES

III. OPTIMAL CONTROL STRATEGY

Linear model predictive control[6],[8] refers to a class of control algorithms that compute a manipulated variable profile by utilizing a linear process model to optimize a linear or quadratic open loop performance objective subject to linear constraints over a future time horizon. The first move of this open loop optimal manipulated variable profile is then implemented. This procedure is repeated at each control interval with the process measurements used to update the optimization problem. MPC is a control algorithm based on solving an online optimal control problem. A receding horizon approach is used, which can be summarized in the following steps:

- 1) At time k and for the current state $x(k)$; solve, on-line, an open-loop optimal control problem over some future interval, taking in to account of constraints.
- 2) Apply the first step in the optimal control sequence.
- 3) Repeat the procedure at time $(k + 1)$; using the current state $x(k + 1)$.

When $x(k)$ is not directly measured, one can obtain a closed loop solution by replacing $x(k)$ by an estimate $\hat{x}(k)$, provided

by some form of observer. The various MPC algorithms only differ amongst themselves in the model used to represent the process, noise and the cost function to be minimized. They share the common features as

- 1) Process model that is explicitly used to predict the process output for a fixed number of steps in to future.
- 2) A known future reference trajectory.
- 3) Calculation of a future control sequence minimizing a certain objective function (usually quadratic, that involves future process output errors and control increments),
- 4) Receding strategy: at each sampling period only the first control signal of the sequence calculated is applied to a process controlled.

Objective Function

The various MPC algorithms propose different objective functions[9] for obtaining the control law. The general aim is that the future output $y(n+j)$ on the considered horizon should follow a desired reference signal w and at the same time, the control effort, u necessary for doing so should be penalized. The general expression for such an objective function will be min

$$J = \sum_{N_2}^{j=N_1} \delta(j) \left[\hat{y}(n + \frac{j}{n}) - \omega(n+j) \right]^2 + \sum_{N_u}^{j=1} \rho(j) [\Delta u(n+j-1)]^2 \quad (10)$$

In some cases, the above equation also includes weighing on control effort. N_1 and N_2 are the minimum and maximum control horizons and N_u is the control horizon. $\omega(n+j)$ is the future reference trajectory.

IV. NONLINEAR STATE ESTIMATION

This section presents discrete-time EKF[3],[4] for nonlinear state estimation. It considers discrete time dynamics and discrete time measurements. This situation is often encountered in practice. Even if the underlying system dynamics are continuous time, the EKF usually needs to be implemented in a digital computer. This means that there might not be enough computational power to integrate the system dynamics as required in a continuous-time EKF or a hybrid EKF. So the dynamics are often discretized. and then a discrete-time EKF can be used.

Suppose the CSTR system model represented as

$$x_k = f_{(k-1)}(x_{(k-1)}, u_{(k-1)}, \omega_{(k-1)}) \quad (11)$$

$$y_k = h_k(x_k, v_k) \quad (12)$$

state noise

$$\omega_k \sim (0, Q_k) \quad (13)$$

and measurement noise

$$v_k \sim (0, R_k) \quad (14)$$

where x_k , u_k and y_k are system state, input and output respectively. ω_k and v_k are zero mean white noise sequence with variance of Q_k and R_k respectively. We perform a Taylor

series expansion of the state equation around $x_{k-1} = \hat{x}_{k-1}$ and $\omega_{k-1} = 0$ to obtain the following:

$$x_k = f_{k-1}(\hat{x}_{k-1}^+, u_{k-1}, 0) + \frac{\partial f_{k-1}}{\partial x} \Big|_{\hat{x}_{k-1}^+} (x_{k-1} - \hat{x}_{k-1}^+) + \frac{\partial f_{k-1}}{\partial x} \Big|_{\hat{x}_{k-1}^+} \omega_{k-1} \quad (15)$$

$$x_k = f_{k-1}(\hat{x}_{k-1}, u_{k-1}, 0) + F_{k-1}(x_{k-1} - \hat{x}_{k-1}^+) + L_{k-1}\omega_{k-1} \quad (16)$$

$$x_k = F_{k-1}x_{k-1} + [f_{k-1}(\hat{x}_{k-1}^+, u_{k-1}, 0) - F_{k-1}\hat{x}_{k-1}^+] + L_{k-1}\omega_{k-1} \quad (17)$$

$$x_k = F_{k-1}x_{k-1} + \tilde{u}_{k-1} + \tilde{W}_{k-1} \quad (18)$$

F_{k-1} and L_{k-1} are defined by the above equation. The known signal u_k and the noise signal \tilde{W}_k are defined as follows:

$$\tilde{u}_k = f_k(\hat{x}_k^+, u_k, 0) - f_k\hat{x}_k^+ \quad (19)$$

$$\tilde{\omega}_k \sim (0, L_k Q_k L_k^T) \quad (20)$$

We linearize the measurement equation around $x_k = \hat{x}_k^-$ and $v_k = 0$ to obtain

$$y_k = h_k(\hat{x}_{k-1}^-, 0) + \frac{\partial h_k}{\partial x} \Big|_{\hat{x}_{k-1}^-} (x_k - \hat{x}_{k-1}^-) + \frac{\partial h_k}{\partial x} \Big|_{\hat{x}_{k-1}^-} v_k \quad (21)$$

$$y_k = h_k(\hat{x}_{k-1}^-, 0) + H_k(x_k - \hat{x}_{k-1}^-) + M_k v_k \quad (22)$$

$$y_k = H_k x_k + [h_k(\hat{x}_{k-1}^-, 0) - H_k \hat{x}_{k-1}^-] + M_k v_k \quad (23)$$

$$y_k = H_k v_k + z_k + \tilde{v}_k \quad (24)$$

H_k and M_k are defined by the above equation. The known signal z_k and the noise signal \tilde{v}_k are defined as

$$z_k = h_k(\hat{x}_{k-1}^-, 0) - H_k \hat{x}_{k-1}^- \quad (25)$$

$$\tilde{v}_k \sim (0, M_k R_k M_k^T) \quad (26)$$

We have a linear state space system in Eqn 18 and a linear measurement in Eqn 24 That means we can use the standard Kalman filter equations to estimate the state. This results in the following equations for the discrete time extended Kalman filter.

$$P_k^- = F_{k-1} P_{k-1}^+ F_{k-1}^T + L_{k-1} Q_{k-1} L_{k-1}^T \quad (27)$$

$$K_k = P_k^- H_k^T (H_k P_k^- H_k^T + M_k R_k M_k^T)^{-1} \quad (28)$$

$$\hat{x}_k^- = f_{k-1}(\hat{x}_{k-1}^-, u_{k-1}, 0) \quad (29)$$

$$z_k = h_k(\hat{x}_k^-, 0) - H_k \hat{x}_k^- \quad (30)$$

$$\hat{x}_k^+ = \hat{x}_k^- + K_k (y_k - H_k \hat{x}_k^- - z_k) \quad (31)$$

$$\hat{x}_k^+ = \hat{x}_k^- + K_k [y_k - h_k(\hat{x}_k^-, 0)] \quad (32)$$

$$P_k^+ = (I - K_k H_k) P_k^- \quad (33)$$

V. RESULTS & DISCUSSION

This section presents results of simulation using MATLAB. Fig. 2 shows the simulation results for controlling temperature inside the reactor when an MPC with EKF is implemented. Simulation parameters like prediction horizon and control horizon are 50 and 2 respectively. After a setpoint change response reaches final steady value within less than 8 seconds. Results shows good tracking performance when a reference trajectory changes.

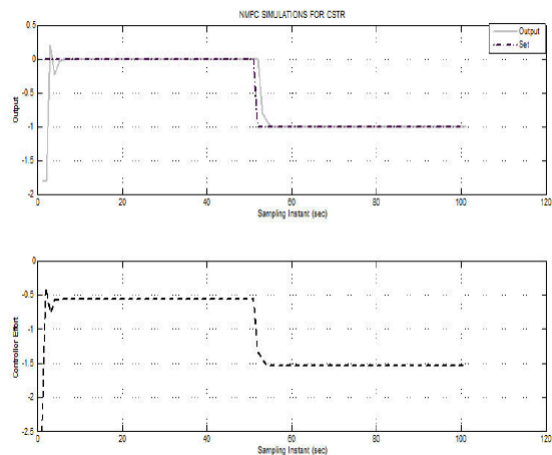


Fig. 2. Simulation results for MPC with Extended Kalman Filter for CSTR

VI. CONCLUSION

Second order mathematical model for CSTR has been developed and dynamic simulation has been performed using it. It can be observed that the optimal control of temperature inside the CSTR is achieved better with the help of MPC strategy compared to conventional control strategies. Nonlinear MPC of CSTR has been demonstrated and response shows that satisfactory setpoint tracking performance with this optimal control strategy has been achieved.

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