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Critical evaluation of non-linear filter configurations for the state estimation of Continuous Stirred Tank Reactor

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ABSTRACT

A systematic approach has been attempted to design a non-linear observer to estimate the states of a non-linear system. The neural network based state filtering algorithm proposed by A.G. Parlos et al. has been used to estimate the state variables, concentration and temperature in the Continuous Stirred Tank Reactor (CSTR) process. (CSTR) is a typical chemical reactor system with complex nonlinear dynamics characteristics. The variables which characterize the quality of the final product in CSTR are often difficult to measure in real-time and cannot be directly measured using the feedback configuration. In this work, the comparison of the performances of an extended Kalman filter (EKF), unscented Kalman filter (UKF) and neural network (NN) based state filter for CSTR that rely solely on concentration estimation of CSTR via measured reactor temperature has been done. The performances of these three filters are analyzed in simulation with Gaussian noise source under various operating conditions and model uncertainties.

1. Introduction

On line estimates of state variables have been considered necessary in diverse applications such as process and controller performance monitoring and state feedback control [13]. State observer can designed to generate an estimate of the state by making use of the relevant process inputs, outputs and mathematical model of the system. The well-known Kalman filter [1] solves the general state estimation problem in stochastic linear system. For linear systems, Kalman filter generate optimal estimates of state from observations. In addition, Kalman filter has become more useful even for very complicated real-time applications and has attracted the attention of chemical engineering community because of recursive nature of its computational scheme. However, for non-linear systems, extended Kalman filter is a natural extension of the linear theory to the non-linear domain through local linearization. There are several variants of the basic EKF, which have been evaluated by various researchers [2]. Many studies in observer design for nonlinear system are based on extended Kalman filter approach, which leads to complex nonlinear algorithm. In spite of good results, there is no a priori guarantee of the convergence and stability of the algorithms. Simon J. Julier proposed an unscented Kalman filter (UKF) [3] for the nonlinear dynamic system. Its use for the state estimation of Continuous Stirred Tank Reactor has been reported in some literatures [4,5,14]. Unlike EKF, it utilizes unscented transform which is a deterministic sampling approach to calculate the current mean and covariance of states and hence called derivative free filter [9,10]. However, the UKF algorithm is more computationally intensive [8] than EKF. A.G. Parlos has proposed a non-adaptive state filtering algorithm for the non-liner dynamic system using neural network. The algorithm presented by the A.G. Parlos et al. is based on the two-step prediction–update approach of the Kalman filter [3]. The use of neural network for state and parameter estimation of CSTR has been well studied [4,5,12]. Structure of the Neural Observer considered in this work differs from EKF in the sense that the function form of state update equation is allowed to be nonlinear and constructed as a neural network, whereas in EKF update state estimate is a linear combination of predicted state estimates and the weighted difference between the actual measurement and the measurement prediction. The main contributions of this work is to implement EKF, UKF and Neural Observer algorithms for the state estimation of Continuous Stirred Tank Reactor and comparative study of the performances under different conditions based on the performance index Mean Square Error (MSE).

2. Mathematical model of CSTR

The first principle model of the continuous stirred tank system and the operating point data [5] (refer Table 1) as specified in the

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Table 1
Steady state operating data of CSTR.

Process variable	Normal operating condition
Measured product concentration (C_A)	0.08235 mol/L
Reactor temperature (T)	441.81 K
Volumetric flow rate (F)	100 L/min
Reactor volume (V)	100 L
Feed concentration (C_{Af})	1 mol/L
Feed temperature (T_f)	350 K
Coolant temperature (T_{co})	350 K
Coolant flow rate (q_c)	100 L/min
Heat of reaction (H)	2e5 cal/mol
Reaction rate constant (k_0)	7.2e10 min^{-1}
Activation energy term (E/R)	9980 K
Heat transfer term (UA)	7e5 cal/(min K)
Liquid density (ρ, ρ_c)	1000 g/L
Specific heat capacity (C_p, C_{pc})	1 cal/(g K)

Pottman and Seborg paper have been used in the simulation studies [6]. Highly nonlinear CSTR process is very common in chemical and petrochemical plants. In the process considered for simulation study as shown in Fig. 1, an irreversible, exothermic reaction A → B occurs in constant volume reactor that is cooled by a single coolant stream.

The CSTR system has two state variables, namely the temperature and the concentration of the reactor. The process is modeled by the following equations:

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{Af} - C_A) - k_0 C_A \exp\left(\frac{-E}{RT}\right) \quad (1)$$

$$\frac{dT}{dt} = \frac{F}{V}(T_f - T) - \left(\frac{-\Delta H}{\rho C_p}\right) k_0 \ \exp\left(\frac{-E}{RT}\right) C_A + \frac{\rho C_{pc}}{\rho C_p V} q_c \left(1 - \exp\left(\frac{-hA}{\rho C_p q_c}\right)\right)(T_{co} - T) \quad (2)$$

Figs. 3 and 4 show the open loop responses of temperature and concentration of the CSTR for the coolant flow rate variation as shown in Fig. 2. So, it can be concluded that the dynamic behavior of the CSTR process is not the same at different operating points and the process is indeed non-linear.

3. Extended Kalman filter

The well-known Kalman filter [1] solves the state estimation problem in a stochastic linear system. The extended Kalman filter (EKF) is probably the most widely used nonlinear filter. For nonlinear problems, the Kalman Filter is not strictly applicable since linearity plays an important role in its derivation and performance as an optimal filter. The EKF attempts to overcome this difficulty

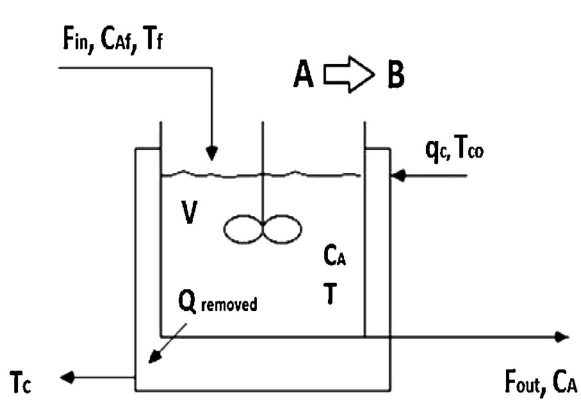

Fig. 1. Continuous Stirred Tank Reactor with cooling jacket.

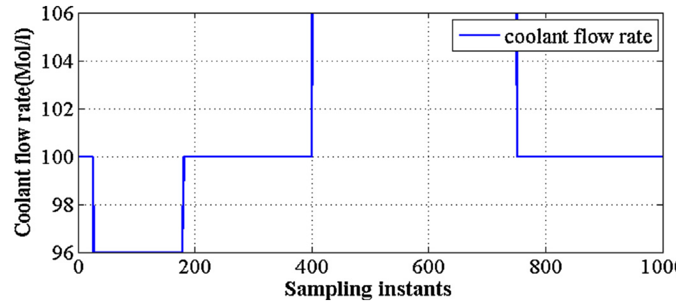

Fig. 2. Variation in coolant flow rate.

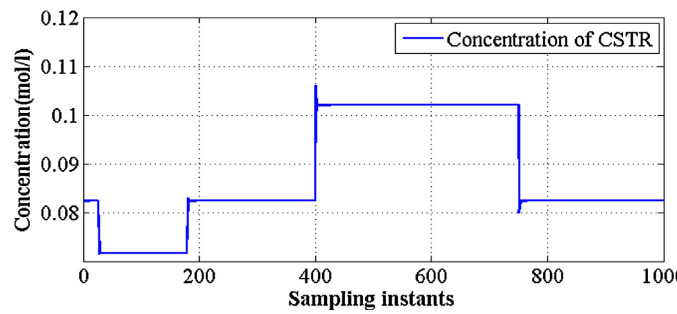

Fig. 3. Open loop response of CSTR (concentration).

by using a linearized approximation where the linearization is performed about the current state estimate. The basic framework for the EKF involves the estimation of the state of a nonlinear dynamic system given by Eqs. (1) and (2).

$$x(k) = \left[x(k-1) + \int_{t_{k-1}}^{t_k} F[x(\tau), u(k)d\tau]\right] + w(k) \quad (3)$$

$$y(k) = H[x(k)] + v(k) \quad (4)$$

In the above equations, $x(k)$ represents the unobserved state of the system, $u(k)$ is a known exogenous input and $y(k)$ is the only observed signal. We have assumed $w(k)$ and $v(k)$ as zero mean Gaussian white noise sequences with covariance matrices Q and R respectively. The symbols F and H represent an n-dimensional function vector and are assumed known. EKF involves the recursive estimation of the mean and covariance of the state under maximum likelihood condition. The function F can be used to compute the predicted state from the previous estimate and similarly the function H can be used to compute the predicted measurement from the predicted state. However, F and H cannot be applied to the covariance directly. Instead a matrix of partial derivatives (Jacobian) is computed at each time step with current predicted state and evaluated. This process essentially linearizes the non-linear function

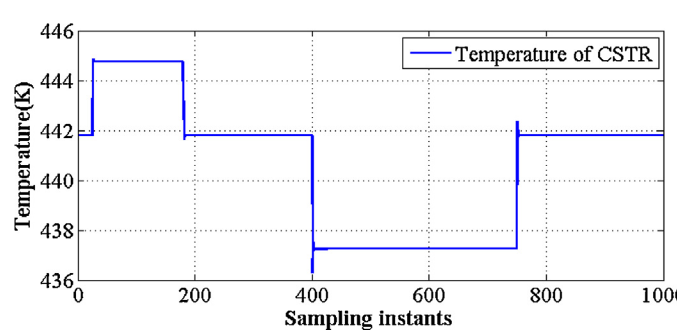

Fig. 4. Open loop response of CSTR (temperature).