SOFT SENSOR BASED NONLINEAR CONTROL OF A CHAOTIC REACTOR

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Abstract: Control of nonlinear systems exhibiting complex dynamic behavior is a challenging task because such systems present a variety of behavioral patterns depending on the values of physical parameters and intrinsic features. Understanding the behavior of the nonlinear dynamic systems and controlling them at the desired conditions is important to enhance their performance. In this work, a soft sensor based nonlinear control strategy is presented and applied to control a chemical reactor that exhibit multi-stationary unstable behavior, oscillations and chaos. In this strategy, an extended kalman filter is designed to serve as a soft sensor that provides the estimates of unmeasured process states. These states are used as inferential measurements to the nonlinear controller that is designed in the framework of globally linearizing control. The results evaluated for stabilizing the reactor for different conditions including deterministic and stochastic disturbances show the better performance of the soft sensor based nonlinear control strategy over that of a PID controller with modified feedback mechanism.

Keywords: Soft Sensor; extended Kalman filter; nonlinear state estimation; chaotic behavior; geometric controller

1. INTRODUCTION

Control of nonlinear systems exhibiting complex dynamic behavior is a challenging task because such systems present a variety of behavioral patterns depending on the values of their physical parameters and intrinsic features. Depending on the parameter values, these systems can operate at steady state or present oscillatory and chaotic motions. In case of chemical reactors, such unconventional behavior can be attributed to some sort of nonlinear interaction between several quantities that can be stored or sometimes inter-converted within the system. The oscillatory and chaotic phenomenon displayed by the chemically reacting systems has desirable as well as undesirable features. The desirable feature of chaos is that it enhances mixing and chemical reactions and provides a vibrant mechanism for transport of heat and mass. On the other hand, the intrinsic features of the reacting systems with the interactive influence of chemical or thermal energy may cause irregular dynamic behavior leading to degraded performance. In such situations, chaos is considered as undesirable and should be avoided. The presence of chaotic behavior in chemical reactors has been demonstrated theoretically and experimentally by several researchers [Uppal et al. (1976); Schimitsch et al. (1979); Wu (2000); Blanco and Bandoni (2007)]. Understanding the dynamic behavior of the chaotic reactor and controlling it under stable operating conditions is important to enhance the performance of the reactor. Various methods including a proportional-Integral (PI) controller [Pellegrini and Biardi (1990)] and a modified PI/PID controller [Bandyopadhyay et al. (1997)] have been used for controlling and operating the chaotic reactors under favorable conditions. However, the complex nature of dynamical systems severely limits the use of conventional linear controllers to provide the desired operating performance. Therefore, advanced control strategies have become an important part of control structure. But most advanced controllers rely on mathematical models of the process incorporating process state variable information in controller formulation. In most systems, the state variables desired by the controller can not be easily available through measurement or available with large measurement delays. Such timely unavailable state variables may restrict the implementation of advanced model based controllers for nonlinear systems. If such inaccessible or non-measurable state variables can be made available either by hard sensing or soft sensing techniques, The nonlinear model based controllers can be implemented effectively. The measurement problems and the delays associated with the hard sensors have led to the development of soft sensors as alternative measurement tools. Model based estimation methods such as extended versions of Kalman filters / nonlinear observers can serve as soft sensors by means of providing reliable estimates for unmeasured variables in...
nonlinear dynamic systems. The potentiality of model based methods for state estimation have been reported for various systems [Schelur and Schmidt (1993); Venkateswarlu and Gangiah(1992); Sargantanis and Karim (1994); Jana et. al (2006)].

This work presents a soft sensor based nonlinear controller to alter the dynamics of a chaotic chemical reactor and drive the system response to the desired condition. An extended Kalman filter (EKF) is designed and used as a soft sensor to provide the reactor species concentrations that serve as inferential measurements to the nonlinear controller. The controller is designed in the globally linearizing control (GLC) framework of Kravaris and Chung (1987). The sensitivity of the soft sensor is studied with respect to the effect of measurement noise as well as the estimator design parameters. The proposed soft sensor based nonlinear controller is evaluated by applying it for the control of a non-isothermal continuous stirred tank reactor (CSTR) that exhibit multi-stationary unstable behavior, oscillations and chaos. The controller is also studied towards the influence of stochastic and deterministic load disturbances. Further the results of the present control strategy are compared with those of a proportional-integral-derivative (PID) controller that involve modified feedback mechanism.

2. SOFT SENSOR BASED NONLINEAR CONTROL STRATEGY

The strategy consists of an extended Kalman filter (EKF) for estimating unmeasured process variables of a nonlinear system. These estimated states serve as inferential measurements to a globally linearizing controller (GLC) which drives the system response to the desired condition. The schematic of this strategy is shown in Fig. 1.

2.1 Process Representation

The mathematical model of the nonlinear dynamical system can be expressed by the following state space form

\[ x(t) = f(x(t), t) + w(t) \]
\[ x(0) = x_0 \]  
(1)

where \( x(t) \) is \( n \)-dimensional state vector, \( f \) is a nonlinear function of state \( x \) and \( w \) is additive Gaussian noise with zero mean.

The linear measurement relation is given by

\[ y(t_k) = Hx(t_k) + v(t_k) \]  
(2)

The nonlinear measurement model with observation noise can be expressed as

\[ y(t_k) = h(x(t_k)) + v(t_k) \]  
(3)

where \( h \) is a nonlinear function of state \( x \) and \( v \) is the vector of observation noise.

The state vector, \( x(t) \), of (1) can be estimated from the known process measurements, \( y(t_i) \), of (2) using nonlinear estimation techniques. The statistical expectations of the covariance matrices associated with \( x(0), w(t) \) and \( v(t_k) \) are referred as the initial state covariance matrix, \( P_0 \), process noise covariance matrix, \( Q \), and observation noise covariance matrix, \( R \). The matrices \( P_0, Q(t) \) and \( R(t_k) \) are generally selected as estimator design parameters which are used to reflect errors in the initial state, process model and process measurements.

2.2 Extended Kalman Filter (EKF)

State estimation methods based on filtering or observation can deliver reliable on-line estimates for state variables defining a process on the basis of available process knowledge including a dynamic model and the incoming data from process measurement sensors. In this study, an extended Kalman filter is used as a soft sensor to provide the estimates of unmeasurable state variables. By this algorithm, state estimation is carried out through recursive implementation of the prediction and correction equations. More details concerning the EKF for state estimation in nonlinear systems can be referred to elsewhere [Gilles (1987); Venkateswarlu and Jeevan Kumar (2006)].

2.2.1 Prediction equations

By starting with an initial estimate \( x_0 \) and its covariance \( P_0 \) at time \( t_{k-1} \) and no measurements are taken between \( t_{k-1} \) and \( t_k \), the propagating expressions for the estimate and its covariance from \( t_{k-1} \) to \( t_k \) are,

\[ \dot{x}(t/t_{k-1}) = f(x(t/t_{k-1}), t) \]
\[ P(t/t_{k-1}) = F(x(t/t_{k-1}), t)P(t/t_{k-1})F'(x(t/t_{k-1}), t) + Q(t) \]  
(4)

where \( F(x(t/t_{k-1}), t) \) is the state transition matrix whose \( i,j \)th element is given by

\[ F(x(t/t_{k-1}), t) = \frac{\partial f(x(t), t)}{\partial x_j(t)} \bigg|_{x(t) = \hat{x}(t/t_{k-1})} \]  
(5)

The solution of the propagated estimate \( x(t/t_{k-1}) \) and its covariance \( P(t/t_{k-1}) \) at time \( t_k \) are denoted by \( x(t_k/t_{k-1}) \) and \( P(t_k/t_{k-1}) \). By using measurements at time \( t_k \), the update estimate \( x(t_k/t_k) \) and \( P(t_k/t_k) \) are computed.
2.2.2 Correction equations

The equations to obtain corrected estimates are
\[
\hat{x}(t_k/t_{k-1}) = \hat{x}(t_k/t_{k-1}) + K(t_k) [y(t_k) - h(x(t_k/t_{k-1}))]
\]
\[
P(t_k/t_{k-1}) = (I - K(t_k)H_k(x(t_k)))P(t_k/t_{k-1})
\]
where
\[
K(t_k) = P(t_k/t_{k-1})H_k^T(x(t_k))P(t_k/t_{k-1})R_k^{-1}
\]

The recursive initial conditions for state and covariance are defined by
\[
\hat{x}(t_1/t_0) = \hat{x}(t_1/t_0)
\]
\[
P(t_1/t_0) = P(t_1/t_0)
\]

3. GLOBALLY LINEARIZING CONTROL (GLC)

The general form of a single input single output (SISO) system with state space description is
\[
x_g = f(x) + g(x)u
\]
\[
y = h(x)
\]
where \(x\) is the vector of \(n\) states, \(u\) is the manipulated input, \(y\) is the measured output, \(f(x)\) and \(g(x)\) are vector functions and \(h(x)\) is the scalar function.

The relative order of the system defined by (13) and (14) is expressed by the following relations:
\[
L_g L_f^{-k} h(x) = 0, k < r - 1
\]
\[
L_g L_f^{-r} h(x) \neq 0
\]
where \(r\) represents the relative order of the system and \(L_f h(x)\) is the Lie derivative of the scalar function \(h(x)\) with respect to the vector function \(f(x)\) with \(L_f h(x) = h(x)\).

Similarly higher order Lie derivatives as well as the Lie derivative of the scalar function \(h(x)\) with respect to the vector function \(g(x)\), and then with respect to the vector function \(g(x)\) can be defined. The relative order defined by (15) and (16) represents the number of times the output \(y\) must be differentiated with respect to time so that the input \(u\) appears explicitly. According to (15) and (16), the first \(r\) time derivatives of the output \(y\) can be expressed as
\[
y^k = L_f^k h(x) ; 0 \leq k \leq r - 1
\]
\[
y^r = L_f^r h(x) + L_g L_f^{-r+1} h(x)u
\]
where
\[
y' = \frac{d^r y(t)}{dt^r}
\]

The GLC approach has been proposed by Kravaris and Chung (1987) for control affine systems and is based on input-output linearization through the use of static state feedback and coordinates transformations. In this approach, a new input \(\nu\) for the controller is defined as
\[
u = \sum_{k=0}^{r} \beta_k \frac{d^k y}{dt^k} = \beta_0 y + \beta_1 y^{(1)} + \ldots + \beta_{r-1} y^{(r-1)} + \beta_r y^{(r)}
\]
From (17), (18) and (19) it follows that
\[
u = \beta_0 h(x) + \beta_1 L_f h(x) + \ldots + \beta_{r-1} L_f^{r-1} h(x) + \beta_r L_f^{r} h(x) + L_g L_f^{-1} h(x)u
\]
\[
= \sum_{k=0}^{r} \beta_k L_f^k h(x) + \beta_r L_g L_f^{-1} h(x)u
\]
By rearranging (20)
\[
u - \sum_{k=0}^{r} \beta_k L_f^k h(x) = \beta_r L_g L_f^{-1} h(x)u
\]
When the poles of the \(\nu-y\) system are appropriately placed (far left in the complex plane), one can use an external PI loop to force the output \(y(t)\) to track a given desired trajectory \(y_d(t)\):
\[
u = k_c \left[ \int (y_d - y) dt + \frac{1}{\tau_i} \int (y_d - y) dt \right]
\]
The GLC structure is then expressed as
\[
u = \frac{k_d \int (y_d - y) + \frac{1}{\tau_i} \int (y_d - y) dt}{\beta_r L_g L_f^{-1} h(x)}
\]
The values of the constants \(\beta_0, \beta_1, \beta_2, \ldots, \beta_r\) and the proportional \((k_c)\) and integral terms\((\tau_i)\) are chosen so that the roots of the characteristic equation has negative real parts. The EKF in conjunction with the process model provides the states, which are used in GLC to compute the control input.

4. CHAOTIC CSTR SYSTEM

Consider the dynamics of a non-isothermal, irreversible, first order series reaction \(A \rightarrow B \rightarrow C\) in a CSTR with control action and load disturbances as governed by the following
dimensionless mass and energy balance equations [Bandyopadhyay et al., 1997]:

\[
\frac{dx_1}{dt} = 1 - x_1 - Da x_1 \exp[x_3/f + \varepsilon_A x_3] + d_1
\]

\[
\frac{dx_2}{dt} = -x_2 + Da x_1 \exp[x_3/f + \varepsilon_A x_3]
\]

\[
= - Da S x_2 \exp[x_3/f + \varepsilon_A x_3] \]

\[
\frac{dx_3}{dt} = -x_3 + B Da x_1 \exp[x_3/f + \varepsilon_A x_3] - \beta(x_3 - x_3^c) + \beta u_t + d_3
\]

The variables \(x_1\) and \(x_2\) denote the dimensionless concentrations of species A and B respectively, and \(x_3\) is the dimensionless temperature. The parameter \(x_3^c\) represents the reactor coolant temperature. An externally manipulated variable \(u_t\) can be defined to denote a measure of the deviation in the coolant temperature from the reference value \(x_3^c\). The notation \(d_1\) and \(d_2\) denote the load disturbances in feed compositions and \(d_3\) represents the load disturbance in the reactor temperature. The system represented by the above equations exhibit multi-stationary behavior, oscillations and chaos for the parameter values shown in Table 1.

### Table 1 Characterization of steady states

<table>
<thead>
<tr>
<th>Set No.</th>
<th>Parameter values</th>
<th>(x_1^s)</th>
<th>(x_2^s)</th>
<th>(x_3^s)</th>
<th>Stability</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>(Da=0.06,) (S=0.0005,) (\varepsilon_x=0, k=1,) (\alpha=0.426,) (\beta=7.7, B=55.0)</td>
<td>0.0378</td>
<td>0.9501</td>
<td>6.0500</td>
<td>Unstable</td>
</tr>
<tr>
<td>II</td>
<td>(Da=0.26,) (S=0.5, \varepsilon_x=0,) (k=1, \alpha=0.426,) (\beta=7.7, B=57.77)</td>
<td>0.0729</td>
<td>0.1259</td>
<td>3.8900</td>
<td>Stable, limit cycle</td>
</tr>
<tr>
<td>III</td>
<td>Same as Set II except (\beta=7.9999)</td>
<td>0.0819</td>
<td>0.1391</td>
<td>3.7627</td>
<td>Chaotic</td>
</tr>
</tbody>
</table>

### 5. DESIGN OF SOFT SENSOR BASED NONLINEAR CONTROLLER

The chaotic CSTR system is used as a simulation test bed to design the soft sensor based nonlinear controller. The schematic of the soft sensor based nonlinear control of chemical reactor is shown in Fig. 2.

#### 5.1 Soft sensor design

The nonlinear dynamic model of the reactor system in its dimensionless form is used in conjunction with the temperature measurements to estimate the reactor species concentrations. The design of soft sensor involves the following components:

**State vector**

The chemical species concentrations and the temperature define the state vector as

\[ x = [x_1 \ x_2 \ x_3]^T \]

**State transition matrix**

The elements \(f_{ij}\) of the state transition matrix, \(F\) are computed by taking the partial derivatives of \(f(x)\) defined by (24)-(26) with respect to the state vector:

\[ F = \begin{bmatrix} f_{11} & f_{12} & f_{13} \\ f_{21} & f_{22} & f_{23} \\ f_{31} & f_{32} & f_{33} \end{bmatrix} \]

**Measurement matrix**

The measurement relation for temperature is

\[ H = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} \]

The temperature state equation, (26) in its discrete form is used as the nonlinear measurement equation, \(h(x)\). The elements of the measurement transition matrix, \(H_s\) are computed by taking the partial derivatives of \(h(x)\) with respect to the state vector:

\[ H_s = [h_{11} \ h_{12} \ h_{13}] \]

All these components are evaluated for chaotic reactor and used with the EKF soft sensor to obtain the measured and unmeasured states of the reactor. The soft sensor uses the temperature data of every sampling time as a measurement and provides the estimates of temperature as well as reactor species concentrations.

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Fig. 2. Schematic of soft sensor based nonlinear control for chaotic CSTR system.
5.2 Controller design

The nonlinear geometric controller is designed for the reactor using the GLC framework of Kravaris and Chung (1987), which transforms a nonlinear input/output system into a linear input/output system based on differential geometric principles.

According to (23) the GLC control law for the nonlinear CSTR is obtained as

\[ u_t = \beta_1 x_1 - \beta_2 x_2 + BDx_1 \frac{r_1}{1 + \varepsilon_4 \Delta x_3} - DaBx_3 \frac{r_3}{1 + \varepsilon_4 \Delta x_3} - \beta_3 \]

(27)

The states obtained from the soft sensor are used in the GLC control law to compute the manipulated variable \( u_t \).

6. RESULTS AND DISCUSSION

The reactor system represented by (24) - (26) exhibits multi-stationary behavior, oscillations and chaos for the given parameter values shown in Table 1. For parameter set I, the system shows unstable steady state, whereas parameter sets II and III, the system exhibits limit cycle oscillations and chaotic behavior, respectively. The temperature data used for state estimation are obtained through numerical integration of the model equations using Gear’s method with a sampling time of 0.0001 units.

The performance of the EKF soft sensor is evaluated by considering different cases of process parameter values shown in Table 1. The results in Fig. 3 represent the phase plane plots of the actual and estimated states of CSTR corresponding to set III. In order to represent the realistic situation, the temperature state is corrupted with random Gaussian noise having a mean 0 and standard deviation 0.25. Fig. 4 shows the actual and estimated concentration profiles corresponding to set III in the presence of stochastic noise in temperature measurement obeying Gaussian distribution. In all the cases, the estimated states are in close resemblance with the actual states. These results thus confirm the better suitability of the method of EKF as a soft sensor for state estimation in chaotic chemical reactors.

A nonlinear geometric controller described in the earlier section is designed and applied to control the reactor under different operating conditions. The states provided by the soft sensor are used as inferential measurements to the GLC controller. The results of the nonlinear controller are also compared to a modified PID controller. The tuning parameters involved in the nonlinear geometric controller and the PID controller are selected appropriately.

The nonlinear controllers are applied with the objective of stabilizing the system at unique unstable steady state responsible for the chaotic motion. In this objective, the controller has to stabilize the chaotic trajectory shown in Fig.3 exactly at the corresponding unique unstable steady state.

For simulating control actions, the parameter set III with the set conditions in Table 1 is used. Figs. 5 & 6 show the process output and controller output plots of modified PID and nonlinear geometric controllers, respectively. These plots indicate that the controllers fulfill the objective of stabilizing chaotic motion at the unstable steady state without allowing any offset. The nonlinear controller has shown better stabilization over PID controller.

http://www.ifac-papersonline.net (DOI: 10.3182/20090921-3-TR-3005.00093)
The controllers are also evaluated by applying them for controlling the system at unstable steady state responsible for chaotic motion in the presence of deterministic and stochastic load disturbances. To realize this objective, the parameter set III is used with the arbitrary initial values \(x_{10}=0.08, \ x_{20}=0.103, \ x_{30}=3.654\) and the set conditions shown in Table 1 with the deterministic disturbance \(d_3=1.0\). The results of nonlinear controller for this case are shown in Fig. 7.

The nonlinear controller performance with the above initial values and set conditions is also evaluated for a stochastic load disturbance generated through random Gaussian noise of zero mean and a standard deviation of 0.25. The results of modified PID controller and nonlinear controller for this case are shown in Figs. 8 and 9.
7. CONCLUSIONS

An extended Kalman filter (EKF) is presented as a soft sensor to estimate the states of a chemical reactor that exhibit multi-stationary unstable behavior, oscillations and chaos. The results evaluated for different conditions show that the EKF soft sensor can be reliably applied for online estimation of unknown states in complex dynamic systems. A nonlinear geometric controller supported by the soft sensor is designed and applied for the control of the chemical reactor. The results demonstrate the effectiveness of the proposed soft sensor based strategy for controlling complex dynamic systems.

REFERENCES


