

Soft Sensor for Inputs and Parameters Using Nonlinear Singular State Observer in Chemical Processes^{*}

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Abstract Chemical processes are usually nonlinear singular systems. In this study, a soft sensor using nonlinear singular state observer is established for unknown inputs and uncertain model parameters in chemical processes, which are augmented as state variables. Based on the observability of the singular system, this paper presents a simplified observability criterion under certain conditions for unknown inputs and uncertain model parameters. When the observability is satisfied, the unknown inputs and the uncertain model parameters are estimated online by the soft sensor using augmented nonlinear singular state observer. The riser reactor of fluid catalytic cracking unit is used as an example for analysis and simulation. With the catalyst circulation rate as the only unknown input without model error, one temperature sensor at the riser reactor outlet will ensure the correct estimation for the catalyst circulation rate. However, when uncertain model parameters also exist, additional temperature sensors must be used to ensure correct estimation for unknown inputs and uncertain model parameters of chemical processes.

Keywords soft sensor, state observer, nonlinear singular system, unknown inputs, uncertain model parameters, riser reactor of fluid catalytic cracking unit

1 INTRODUCTION

In chemical processes, the operation and control depend on many key input variables that are difficult to measure in real-time with current process instruments. Soft sensor is an effective method for real-time measurement of unmeasurable variables and gradually receives more attention.

At present, the research on soft sensor is mainly on the modeling of soft sensor, establishing mathematical relation between the primary variables unmeasurable and the secondary variables easy to be measured. The modeling of soft sensor includes the extended Kalman filter [1], the high-gain observer [2], the artificial neural network [3], the hybrid fuzzy c-means algorithm and support vector machine [4], the independent component analysis and partial least squares [5], and the relevance vector machine [6]. The multiple model method [7, 8] and local learning adaptive model [9] are also used in the modeling of soft sensor. Because of the complexity and uncertainty of chemical processes, errors are inevitably present. Many input variables are unmeasurable and model parameters are uncertain in chemical processes, so the soft sensor for unknown inputs and uncertain model parameters can be corrected only on-line by secondary variables easy to be measured. The form of soft sensor using output correction of secondary variables will be similar to state observer. When the unknown inputs [10–13] and the uncertain model parameters [14, 15] are augmented as state variables, the soft sensor based on state observer could be built to estimate the unknown inputs and correct the uncertain model parameters online.

The first-principle models of chemical processes are composed of both algebraic and differential equations (DAE), which are called singular systems. Mass and energy balance equations are differential equations, while the equations for mass and energy transfer rate, chemical reaction rate, and thermodynamic state are algebraic equations. In some chemical processes, such as in a riser reactor of fluid catalytic cracking unit (FCCU), the dynamic response of component mass percents is much faster than that of temperature. Hence, the former can be assumed as a quasi-steady state, and mass balance equations become algebraic equations to form another singular system. In the past two decades, singular systems have been widely studied, including stability and Lyapunov theorem [16], poles assignment [17], state feedback stabilization [18], impulse analysis [19], observability and controllability [20–22], most of which focus on linear singular systems or a specific class of nonlinear singular systems. To build the soft sensor for unknown inputs and uncertain model parameters, the nonlinear singular state observer must be used.

State observer for nonlinear singular systems is important in the singular system control theory. The study on the state observer of a linear singular system is mainly focused on the Luenberger observer [23–25] and has been studied intensively. However, state observer for nonlinear singular systems is much more complicated. Zimmer and Meier [26] studied the problem of observing the state of continuous nonlinear descriptor systems in quasilinear form and presented a method to construct a state observer. Lan *et al.* [27] presented the state observer for bilinear descriptor systems by poles assignment method and the observe

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error was Lyapunov asymptotically stable. For a class of Lipschitz nonlinear singular systems, Lu and Ho [28] constructed both types of full-order and reduced-order observers by a unified linear matrix inequality approach. Darouach and Boutat-Baddas gave the sufficient conditions for the existence of observers using linear matrix inequalities formulation [29] and the H_∞ observers for Lipschitz nonlinear singular systems [30]. Xu *et al.* [31] transformed a singular system to a normal system after the linearization of nonlinear singular system at current operating point and designed the state observer according to normal system. In this study, we directly design the singular state observer according to singular system. Using the method of adaptive observer [32, 33], the output feedback matrix of state observer is obtained online through poles assignment of the linear parameter-varying singular system at current operating point of the nonlinear singular system.

When unknown inputs and uncertain model parameters are augmented as state variables, state observation will become more difficult as the system dimension increases. Waldruff *et al.* [34] and Vandenberg *et al.* [35] used the observability matrix of linearized systems to analyse system observability and modified sensor placement.

The present paper presents a simplified observability criterion under certain conditions for unknown inputs and uncertain model parameters. When observability is satisfied, a soft sensor using augmented nonlinear singular state observer is designed for unknown inputs and uncertain model parameters.

2 AUGMENTATIONS OF UNKNOWN INPUTS AND UNCERTAIN MODEL PARAMETERS

In the nonlinear singular system given by

$$\begin{cases} E\dot{x} = f(x, u, v, p) \\ y = Cx \end{cases} \quad (1)$$

$x \in \mathbf{R}^n$ is the state, $y \in \mathbf{R}^l$ is the measured output, $u \in \mathbf{R}^{m_0}$ is the known control input, $v \in \mathbf{R}^{m_1}$ is the unknown input, $p \in \mathbf{R}^{m_2}$ is the uncertain model parameter, and $f(\cdot)$ is the n -dimensional mapping function of the state and is assumed to be smooth. The matrix $E \in \mathbf{R}^{n \times n}$ may be singular, and $\text{rank}(E) = q < n$.

In general real processes, $E = \text{diag}(I_q, 0)$, and a more practical form is given by

$$\begin{cases} \dot{x}_1 = f_1(x_1, x_2, u, v, p) \\ 0 = f_2(x_1, x_2, u, v, p) \\ y = C_1 x_1 + C_2 x_2 \end{cases} \quad (2)$$

where $x_1 \in \mathbf{R}^q$ is the differential vector and $x_2 \in \mathbf{R}^{n-q}$ is the algebraic vector.

Chemical processes usually belong to an index-one singular system, which implies that

$$\text{rank}\left(\frac{\partial f_2(x_1, x_2)}{\partial x_2}\right) = n - q$$

To be observed, the unknown input v needs to be augmented as state variables. As Besancon [36] reported, the estimation accuracy of an augmented state observer is independent of the dimension of augmented state variables. Thus the dynamic model of augmented unknown input v is

$$\frac{dv}{dt} = 0 \quad (3)$$

with the initial value $v(t_0) = v_0$.

As the uncertain model parameter is constant, it is augmented as a state variable of one dimension and the dynamic model is

$$\frac{dp}{dt} = 0 \quad (4)$$

with the initial value $p(t_0) = p_0$.

After the unknown inputs and uncertain parameters are augmented as state variables, the augmented system becomes

$$\begin{cases} E_e \dot{x}_e = f_e(x_e, u) \\ y = C_e x_e \end{cases} \quad (5)$$

where $x_e = \begin{bmatrix} v \\ p \\ x \end{bmatrix}$, $f_e = \begin{bmatrix} 0 \\ 0 \\ f(x, u, v, p) \end{bmatrix}$,

$$E_e = \begin{bmatrix} I_{m_1} & 0 & 0 \\ 0 & I_{m_2} & 0 \\ 0 & 0 & E \end{bmatrix}, \text{ and } C_e = [0 \quad 0 \quad C].$$

The linearized form of the augmented system in Eq. (5) is

$$\begin{cases} E_e \dot{x}_e = A_e x_e + B_e u \\ y = C_e x_e \end{cases} \quad (6)$$

where $A_e = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ F & G & A \end{bmatrix}$, $B_e = \begin{bmatrix} 0 \\ 0 \\ B \end{bmatrix}$, $A = \frac{\partial f}{\partial x} \Big|_{x, u, v, p}$, $B = \frac{\partial f}{\partial u} \Big|_{x, u, v, p}$, $F = \frac{\partial f}{\partial v} \Big|_{x, u, v, p}$, and $G = \frac{\partial f}{\partial p} \Big|_{x, u, v, p}$.

3 OBSERVABILITY CRITERION FOR UNKNOWN INPUTS AND UNCERTAIN MODEL PARAMETERS

Based on the observability criterion of singular systems, a simplified observability criterion under certain conditions is presented for unknown inputs and

uncertain model parameters.

Lemma 1 [37] The linear singular system (E, A, C) is observable, if and only if

$$\text{rank} \begin{bmatrix} sE - A \\ C \end{bmatrix} = n, \quad \forall s \in \mathbb{C} \quad (7)$$

and

$$\text{rank} \begin{bmatrix} E \\ C \end{bmatrix} = n \quad (8)$$

Theorem 1 With the assumption that the original system in Eq. (1) is observable at the current operating point, the augmented system in Eq. (5), in which unknown inputs and uncertain model parameters are augmented as state variables, is locally observable at an operating point, if and only if

$$\text{rank} \begin{bmatrix} 0 & 0 & C \\ F & G & A \end{bmatrix} = n + m_1 + m_2 \quad (9)$$

Proof The augmented system in Eq. (5) is locally observable at an operating point, if and only if its linearized system (E_e, A_e, C_e) is observable, such that

$$\text{rank} \begin{bmatrix} sI_{m_1} & 0 & 0 \\ 0 & sI_{m_2} & 0 \\ -F & -G & sE - A \\ 0 & 0 & C \end{bmatrix} = n + m_1 + m_2, \quad \forall s \in \mathbb{C} \quad (10)$$

and

$$\text{rank} \begin{bmatrix} I_{m_1} & 0 & 0 \\ 0 & I_{m_2} & 0 \\ 0 & 0 & E \\ 0 & 0 & C \end{bmatrix} = n + m_1 + m_2 \quad (11)$$

As the original system in Eq. (1) is observable at the current operating point, its linearized system is also observable. Hence, Eq. (11) is obviously satisfied, and Eq. (10) is satisfied, if and only if

$$\text{rank} \begin{bmatrix} 0 & 0 & C \\ F & G & A \end{bmatrix} = n + m_1 + m_2$$

This completes the proof.

The necessary observability conditions for unknown inputs and uncertain model parameters can be further deduced from **Theorem 1**.

Corollary The necessary observability conditions of the augmented system in Eq. (5), in which unknown inputs and uncertain model parameters are augmented as state variables, are

$$\text{rank}[C] = l, \quad l \geq m_1 + m_2$$

and

$$\text{rank}[F] = m_1, \quad \text{rank}[G] = m_2$$

The **Corollary** means that the augmented system

in Eq. (5) will not be observable if the dimension of the unknown inputs plus the dimension of uncertain model parameters $m_1 + m_2$ is larger than the dimension of measured outputs l .

4 SOFT SENSOR USING AUGMENTED NONLINEAR SINGULAR STATE OBSERVER

For the augmented system in Eq. (5), a singular state observer exists as

$$E_e \dot{\hat{x}}_e = f_e(\hat{x}_e, u) + L[y - C_e \hat{x}_e] \quad (12)$$

Based on the singular state observer in Eq. (12), a soft sensor is built to estimate the unknown inputs and uncertain model parameters.

$$\begin{cases} E_e \dot{\hat{x}}_e = f_e(\hat{x}_e, u) + L[y - C_e \hat{x}_e] \\ \hat{y}_0 = C_0(\hat{x}_e) \end{cases} \quad (13)$$

where y_0 is the output of soft sensor, $y_0 = \begin{bmatrix} v \\ p \end{bmatrix}^T$, and

$$C_0 = \begin{bmatrix} I_{m_1} & 0 & 0 & \cdots & 0 \\ 0 & I_{m_2} & 0 & \cdots & 0 \end{bmatrix}.$$

If $e = x_e - \hat{x}_e$ is the estimation error of real states and estimated states, e satisfies the following error equation of the state observer:

$$E_e \dot{e} = f_e(\hat{x}_e + e, u) - f_e(\hat{x}_e, u) - LC_e e \quad (14)$$

Equation (14) shows that an equilibrium point at $e = 0$ exists. If the error equation in Eq. (14) is locally and asymptotically stable at its equilibrium point $e = 0$, the nonlinear singular state observer in Eq. (12) will be convergent.

The linearized form of the error equation in Eq. (14) at $e = 0$ is

$$E_e \dot{e} = (A_e - LC_e)e \quad (15)$$

Lemma 2 [37] If (E, A, C) is observable, a matrix L always exists, which makes the poles set of $(E, A - LC)$ equal any set Λ of q conjugated complex numbers [i.e., $\sigma(E, A - LC) = \Lambda$].

Theorem 2 $x = 0$ is an equilibrium point for the nonlinear singular system $E\dot{x} = f(x)$ and $A = \left. \frac{\partial f}{\partial x} \right|_{x=0}$,

where $f: D \rightarrow R^n$ is continuously differentiable, and D is the neighbourhood near the origin. If (E, A) is stable and impulse-free, the nonlinear singular system $E\dot{x} = f(x)$ is asymptotically stable near the origin.

Proof See Appendix.

Theorem 2 extends the theory of Lyapunov linearization and stability from a normal system to a singular system. On the basis of **Theorem 2**, the following theorem is proposed for the design of a nonlinear singular state observer.

Theorem 3 For the nonlinear singular system $\begin{cases} E\dot{x} = f(x, u) \\ y = h(x) \end{cases}$, if its linearized system (E, A, C) at the operating point is observable, an asymptotically stable singular state observer $E\dot{\hat{x}} = f(\hat{x}, u) + L[y - h(\hat{x})]$ must exist.

Proof The error equation of the singular state observer is

$$E\dot{e} = f(\hat{x} + e, u) - f(\hat{x}, u) - L[h(\hat{x} + e) - h(\hat{x})]$$

Its linearized form at equilibrium point $e = 0$ is

$$E\dot{e} = (A - LC)e$$

From **Lemma 2**, if (E, A, C) is observable, $(E, A - LC)$ can be made stable and impulse-free by choosing L to assign the poles of $(E, A - LC)$ arbitrarily.

From **Theorem 2**, if $(E, A - LC)$ is stable and impulse-free, the error equation of the singular state observer is locally and asymptotically stable at $e = 0$. The singular state observer will be convergent.

This procedure completes the proof.

Hence, if the linearized augmented system (E_e, A_e, C_e) is observable, a singular state observer must exist.

Obviously, the linearized systemic matrix A_e of the augmented system changes with the operating point of the real process, so the feedback gain matrix L of the singular state observer should be adjusted online accordingly to assign the dynamic poles of $(E_e, A_e - LC_e)$ at the appropriate location. Therefore, at each sampling time, the feedback gain matrix L should be refreshed to accommodate the operating point changes through online poles assignment of the linearized system.

The implementation steps for calculating the feedback gain matrix L are as follows.

(1) Linearize the augmented nonlinear singular system in Eq. (5) at the operating point to obtain (E_e, A_e, C_e) . As Eq. (5) is the index-one singular system, (E_e, A_e, C_e) is the second equivalent form of the singular system [37].

$$E_e = \begin{bmatrix} I_{m_1+m_2+q} & 0 \\ 0 & 0 \end{bmatrix}, \quad A_e = \begin{bmatrix} A_{e,11} & A_{e,12} \\ A_{e,21} & A_{e,22} \end{bmatrix},$$

$$C_e = [C_{e,1} \quad C_{e,2}]$$

$$\text{where } A_{e,22} \text{ is non-singular, } A_{e,11} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ F_1 & G_1 & A_{11} \end{bmatrix},$$

$$A_{e,12} = \begin{bmatrix} 0 \\ 0 \\ A_{12} \end{bmatrix}, \quad A_{e,21} = [F_2 \quad G_2 \quad A_{21}], \quad A_{e,22} = [A_{22}],$$

$$C_{e,1} = [0 \quad 0 \quad C_1], \text{ and } C_{e,2} = [C_2].$$

(2) Let $\tilde{E} = E_e^T$, $\tilde{A} = \tilde{A}_e^T$, $\tilde{B} = C_e^T$, and $(\tilde{E}, \tilde{A},$

$\tilde{B})$ be the dual system of (E_e, A_e, C_e) .

$$\dot{\tilde{x}}_1 = \tilde{A}_{11}\tilde{x}_1 + \tilde{A}_{12}\tilde{x}_2 + \tilde{B}_1u,$$

$$0 = \tilde{A}_{21}\tilde{x}_1 + \tilde{A}_{22}\tilde{x}_2 + \tilde{B}_2u$$

where $\tilde{A}_{11} = A_{e,11}^T$, $\tilde{A}_{12} = A_{e,21}^T$, $\tilde{A}_{21} = A_{e,12}^T$, $\tilde{A}_{22} = A_{e,22}^T$, $\tilde{B}_1 = C_{e,1}^T$, and $\tilde{B}_2 = C_{e,2}^T$.

(3) Non-singular matrices Q and P exist.

$$Q = \begin{bmatrix} I_q & 0 \\ -\tilde{A}_{22}^{-1}\tilde{A}_{21} & \tilde{A}_{22}^{-1} \end{bmatrix}, \quad P = \begin{bmatrix} I_q & -\tilde{A}_{12}\tilde{A}_{22}^{-1} \\ 0 & I_{n-q} \end{bmatrix},$$

$$\text{such that } P\tilde{E}Q = \begin{bmatrix} I_{m_1+m_2+q} & 0 \\ 0 & 0 \end{bmatrix}, \quad P\tilde{A}Q = \begin{bmatrix} \bar{A}_1 & 0 \\ 0 & I_{n-q} \end{bmatrix},$$

$$\text{and } P\tilde{B} = \begin{bmatrix} \bar{B}_1 \\ \bar{B}_2 \end{bmatrix}.$$

The system is thus transformed into the first equivalent form of the singular system [37].

$$\dot{\tilde{x}}_1 = \bar{A}_1\tilde{x}_1 + \bar{B}_1u,$$

$$0 = \bar{x}_2 + \bar{B}_2u,$$

where $\tilde{A}_1 = \tilde{A}_{11} - \tilde{A}_{12}\tilde{A}_{22}^{-1}\tilde{A}_{21}$, $\bar{B}_1 = \tilde{B}_1 - \tilde{A}_{12}\tilde{A}_{22}^{-1}\tilde{B}_2$, and $\bar{B}_2 = \tilde{B}_2$.

(4) As (E_e, A_e, C_e) is observable, $(\tilde{E}, \tilde{A}, \tilde{B})$ is controllable and the slow subsystem $(\bar{A}_1, \bar{B}_1)$ is also controllable. On the basis of the state feedback stabilisation controller design method of the normal system, $\bar{K}_1$ can be found to assign the poles of $(\bar{A}_1 - \bar{B}_1\bar{K}_1)$ at the appropriate locations. Then $K = [\bar{K}_1 \quad 0]Q^{-1}$ makes $\sigma(\tilde{E}, \tilde{A} - \tilde{B}K)$ for the designed poles assignments.

(5) With $L = K^T$ as the feedback gain matrix of the state observer,

$$L = Q^{-T} \begin{bmatrix} \bar{K}_1^T \\ 0 \end{bmatrix} = \begin{bmatrix} I_q & \tilde{A}_{21}^T \\ 0 & \tilde{A}_{22}^T \end{bmatrix} \begin{bmatrix} \bar{K}_1^T \\ 0 \end{bmatrix} = \begin{bmatrix} \bar{K}_1^T \\ 0 \end{bmatrix}$$

When the state observer is running, changing the feedback gain matrix L is not continuous but discrete. During each sampling period, the feedback gain matrix L remains unchanged, and the state observer will run for a sampling period. After the sampling period is finished, the feedback gain matrix L will be calculated following Steps (1) to (5), and running the next sampling period will begin. For the convergence of numerical simulation, the sampling period h and the poles need to assign λ_j , $j = 1, 2, \dots, m_1 + m_2 + q$ which

should satisfy the condition $h < \frac{2}{|\lambda_{\max}|}$.

5 CASE STUDY

The dynamic model [38] of the riser reactor of FCCU (fluid catalytic cracking unit) is given by

$$\begin{aligned} \frac{dT_{ra,i}}{dt} &= -\frac{N}{S_T} \left(\frac{1}{1+F} \right) (T_{ra,i} - T_{ra,i-1}) - \left(\frac{A}{1+F} \right) \left(\frac{G_C}{F_O} \right) \times \\ &\quad \left\{ [\Delta H_{AR} k_{A0} y_{A,i} + \Delta H_{DR} k_{D0} y_{D,i} + \Delta H_{NR} k_{N0} y_{N,i}] - \right. \\ &\quad \left. \Delta H_{AA} [\nu_{AC} k_{A0} y_{A,i} + \nu_{DC} k_{D0} y_{D,i}] \right\} \exp \left(-\frac{E_A}{RT_{ra,i}} \right) p_{ra} \varphi_i \\ y_{A,i} &= y_{A,i-1} - \frac{S_T}{N} \left(\frac{G_C}{F_O} \right) k_{A0} y_{A,i} \exp \left(-\frac{E_A}{RT_{ra,i}} \right) p_{ra} \varphi_i \\ y_{D,i} &= y_{D,i-1} + \frac{S_T}{N} \left(\frac{G_C}{F_O} \right) \times \\ &\quad [\nu_{AD} k_{A0} y_{A,i} - k_{D0} y_{D,i}] \exp \left(-\frac{E_A}{RT_{ra,i}} \right) p_{ra} \varphi_i \\ y_{N,i} &= y_{N,i-1} + \frac{S_T}{N} \left(\frac{G_C}{F_O} \right) [\nu_{AN} k_{A0} y_{A,i} + \\ &\quad \nu_{DN} k_{D0} y_{D,i} - k_{N0} y_{N,i}] \exp \left(-\frac{E_A}{RT_{ra,i}} \right) p_{ra} \varphi_i \\ y_{G,i} &= y_{G,i-1} + \frac{S_T}{N} \left(\frac{G_C}{F_O} \right) [\nu_{AG} k_{A0} y_{A,i} + \\ &\quad \nu_{DG} k_{D0} y_{D,i} + \nu_{NG} k_{N0} y_{N,i}] \exp \left(-\frac{E_A}{RT_{ra,i}} \right) p_{ra} \varphi_i \\ C_{ra,i} &= C_{ra,i-1} + \frac{S_T}{N} [\nu_{AC} k_{A0} y_{A,i} + \\ &\quad \nu_{DC} k_{D0} y_{D,i}] \exp \left(-\frac{E}{RT_{ra,i}} \right) p_{ra} \varphi_i \\ \varphi_i &= \varphi_{i-1} - \frac{S_T}{N} k_{\varphi 0} \exp \left(-\frac{E_{\varphi}}{RT_{ra,i}} \right) p_{ra} y_{A,i} \varphi_i \\ i &= 1, 2, \dots, N \end{aligned}$$

The dynamic model can be rewritten as

$$\begin{cases} \dot{\mathbf{x}}_1 = \mathbf{f}_1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{u}, \mathbf{v}, \mathbf{p}) \\ 0 = \mathbf{f}_2(\mathbf{x}_1, \mathbf{x}_2, \mathbf{u}, \mathbf{v}, \mathbf{p}) \\ \mathbf{y} = \mathbf{C}_1 \mathbf{x}_1 \end{cases}$$

where $\mathbf{x}_1 = [T_{ra,1} \ \dots \ T_{ra,N}]^T$, $\mathbf{x}_2 = [y_{A,1} \ y_{D,1} \ y_{N,1} \ y_{G,1} \ C_{ra,1} \ \phi_1 \ \dots \ y_{A,N} \ y_{D,N} \ y_{N,N} \ y_{G,N} \ C_{ra,N} \ \phi_N]^T$, $\mathbf{u} = [F_O \ T_{ra,0}]^T$, $\mathbf{v} = [G_C]^T$, $\mathbf{p} = [k_{A0}]^T$, $\mathbf{f}_1(\cdot)$ signifies the differential equations, and $\mathbf{f}_2(\cdot)$ represents the algebraic equations.

The riser reactor of FCCU is a typical index-one nonlinear singular system. The catalyst circulation rate G_C is the main unknown input. The pre-exponential factor of reaction rate constant of crude oil k_{A0} is always influenced by oil material properties and needs to be modified by real process data, which is considered as the main uncertain model parameter. N is the number of FCCU riser segments, and $N = 4$ here.

Firstly, the dynamic model of the FCCU riser reactor is assumed to be accurate without uncertain model parameters, and only G_C is unknown. G_C is thus augmented as one state variable. Only one temperature sensor is present at the outlet of the FCCU riser, that is

$$\mathbf{C}_1 = [0 \ 0 \ 0 \ 1]$$

The dimension of the unknown inputs is equal to the dimension of the measurable output, which satisfies the necessary observability condition of the **Corollary**. At the same time, $n = 7 \times N = 28$, $m_1 = 1$, $m_2 = 1$, and

$$\text{rank} \begin{bmatrix} 0 & 0 & \mathbf{C} \\ \mathbf{F} & \mathbf{G} & \mathbf{A} \end{bmatrix} = 29$$

so **Theorem 1** is also satisfied.

The soft sensor using augmented singular state observer is designed to estimate G_C . To examine how the assigned poles of state observer to influence the observation results, we take two set of assigned poles of state observer into account, with the first poles set of $[-0.68, -0.68, -0.68, -0.68, -0.68]$ and the second poles set of $[-0.4, -0.4, -0.4, -0.4, -0.4]$. To study the influence of signal forms of the unknown input, we consider G_C of a square signal or a sinusoidal signal. Fig. 1 (a) shows the curves of the real values and estimated values of G_C when the unknown input is a square signal, while Fig. 1 (b) shows those when the unknown input is a sinusoidal signal. The estimated values of G_C are convergent to the real values. When the assigned poles of state observer are more negative, the convergence rate of state observer is quicker.

To investigate the adaptive capacity for stochastic noise, we add the normally distributed stochastic noise on the signal of the unknown input. Fig. 2 shows the curves of the real values and estimated values of G_C with two poles set for the unknown input of a square signal or a sinusoidal signal with stochastic noise added. The simulation indicates that the impact of stochastic noise is very limited and the state observer with more negative assigned poles is also of the faster convergence rate even under the condition of stochastic noise.

Table 1 shows the mean errors of G_C during the whole dynamic processes of state observer. The mean error with noise is slightly larger than that without noise and the more negative assigned poles gives less mean error.

Secondly, both unknown input and uncertain model parameter exist in the dynamic model of the FCCU riser reactor, where G_C is the unknown input and k_{A0} is the uncertain model parameter. If only one temperature sensor is present at the outlet of the FCCU riser as before, that is $\mathbf{C}_1 = [0 \ 0 \ 0 \ 1]$, the

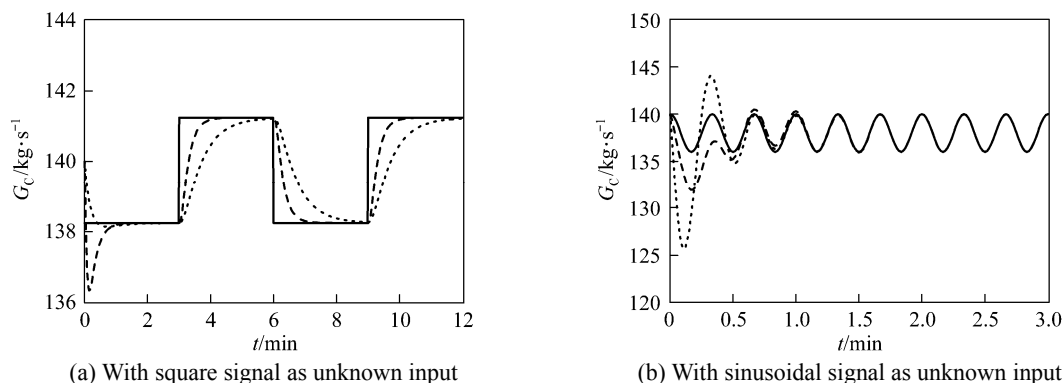


Figure 1 Catalyst circulation rate for unknown input without noise

— real value; - - - estimated value of the first poles set; estimated value of the second poles set

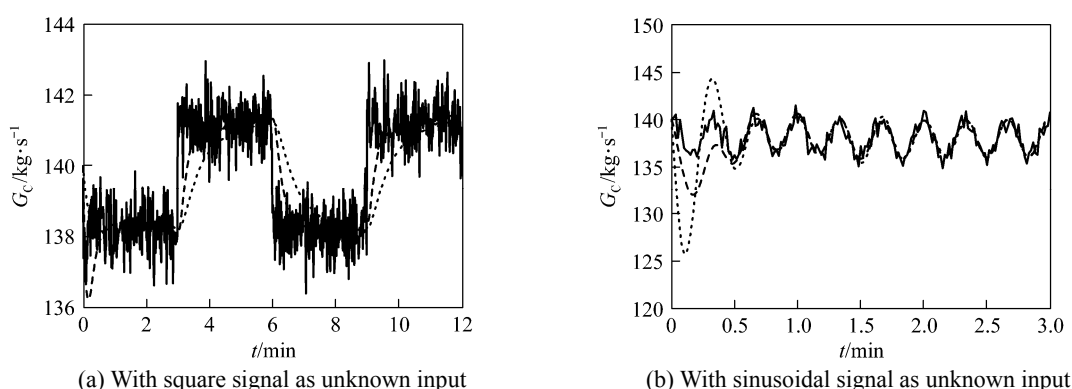


Figure 2 Catalyst circulation rate for unknown input with noise

— real value; - - - estimated value of the first poles set; estimated value of the second poles set

Table 1 The mean errors of the catalyst circulation rate/kg.s⁻¹

Scenarios	Square signal		Sinusoidal signal	
	No noise	Noise	No noise	Noise
the first poles set	0.306	0.357	0.562	0.630
the second poles set	0.604	0.618	0.824	0.988

$$C_1 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

The dimension of the unknown input plus the dimension of the uncertain model parameter is equal to that of measured outputs. The necessary observability condition of the **Corollary** is satisfied. At the same time, $n = 7 \times N = 28$, $m_1 = 1$, $m_2 = 1$, and

$$\text{rank} \begin{bmatrix} 0 & 0 & C \\ F & G & A \end{bmatrix} = 30$$

so **Theorem 1** is satisfied.

The soft sensor using augmented singular state observer is designed to estimate both unknown input and uncertain model parameter with the temperature sensor in the middle of the riser reactor added. To study the impact of the assigned poles of state observer, we also consider two set of assigned poles of state observer, the first poles set is $[-0.7, -0.7, -0.7, -0.7, -0.1, -0.1]$ and the second set is $[-0.5, -0.5, -0.5, -0.5, -0.05, -0.05]$. To study the influence of signal forms of the unknown input, we also consider G_C of a square signal or a sinusoidal signal. Fig. 3 shows the curves of the real values and estimated values of G_C and Fig. 4 shows the curves of k_{A0} . The

dimension of the unknown input plus the dimension of the uncertain model parameter is 2, which is larger than that of measured outputs for the only one temperature sensor at the outlet of the FCCU riser. It will not satisfy the necessary observability conditions of the **Corollary**. At the same time, $n = 7 \times N = 28$, $m_1 = 1$, $m_2 = 1$, and

$$\text{rank} \begin{bmatrix} 0 & 0 & C \\ F & G & A \end{bmatrix} = 29 < 30$$

so **Theorem 1** is not satisfied either.

More measure points should be added. If one temperature sensor is placed in the middle of the riser reactor and another is at the outlet, the dimension of the measured outputs becomes 2, that is

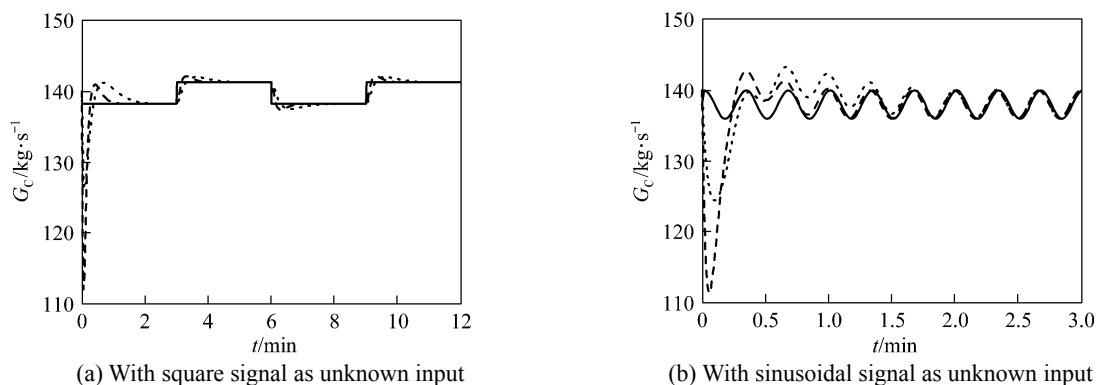


Figure 3 Catalyst circulation rate for unknown input and uncertain model parameter without noise

— real value; - - - estimated value of the first poles set; estimated value of the second poles set

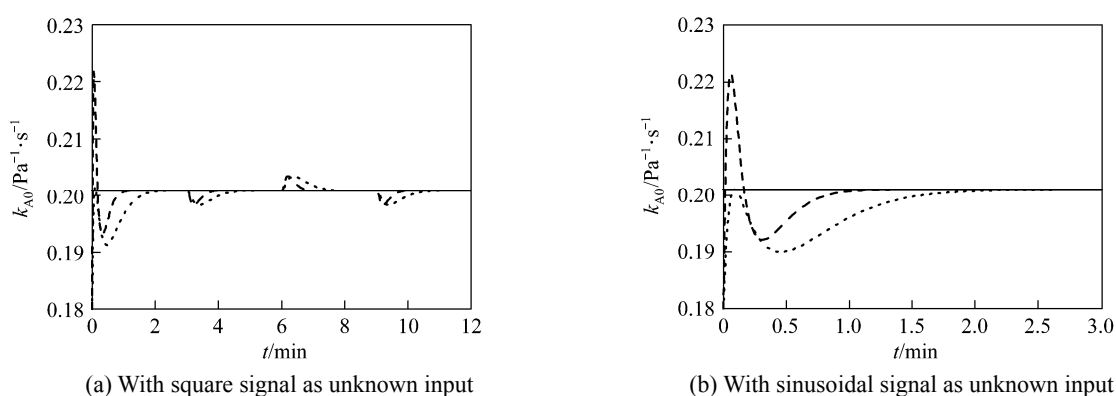


Figure 4 Reaction rate constant pre-exponential factor of crude oil without noise

— real value; - - - estimated value of the first poles set; estimated value of the second poles set

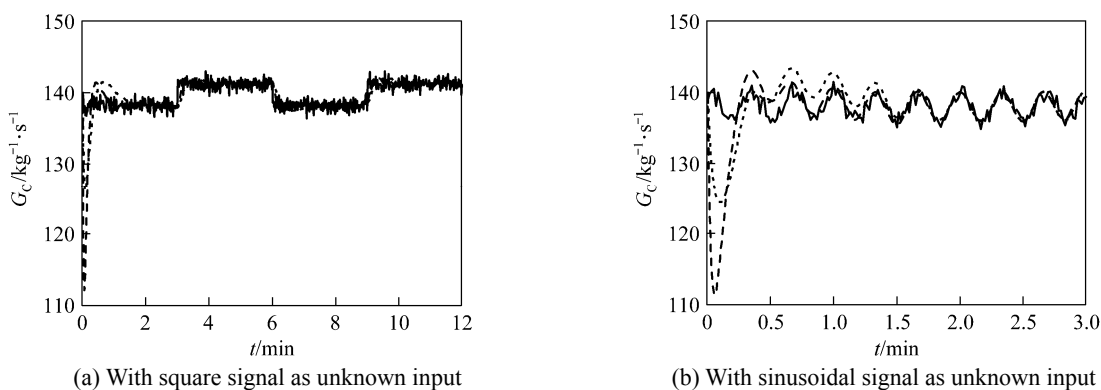


Figure 5 Catalyst circulation rate for unknown input and uncertain model parameter with noise

— real value; - - - estimated value of the first poles set; estimated value of the second poles set

estimated values of G_C are convergent to the real values, and even if an initial estimation error is encountered for k_{A0} , the estimated value converges to the real value through the online modification of the state observer when it is augmented as a state variable. The assigned poles of state observer are relevant to the convergence rate of state observer. The more negative the assigned poles, the faster the convergence rate.

With both the unknown input and uncertain model parameter, we add the normally distributed stochastic

noise on the signal of the unknown input. Fig. 5 shows the curves of the real values and estimated values of G_C with stochastic noise and Fig. 6 shows the curves of k_{A0} . The estimated values of G_C and k_{A0} converge to the real values and the state observer with more negative assigned poles has faster convergence rate even under the influence of stochastic noise.

Tables 2 and 3 show the mean errors of G_C and k_{A0} in the whole dynamic process of state observer. The mean error with noise is very close to the mean

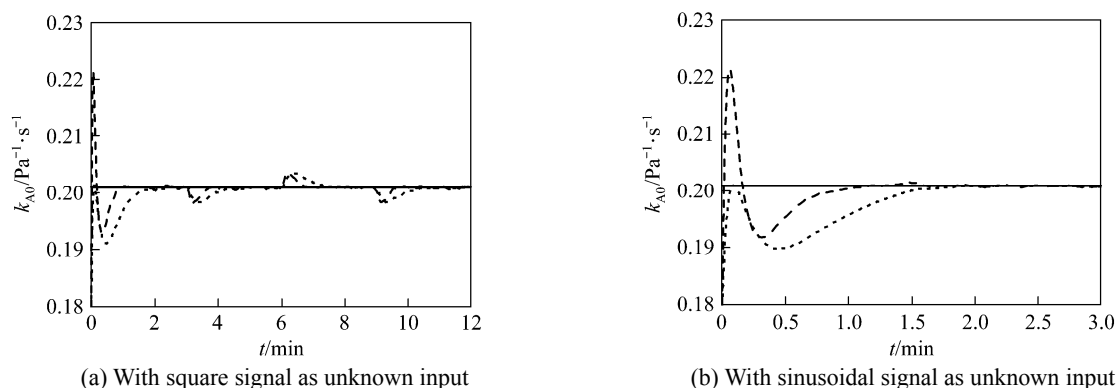


Figure 6 Reaction rate constant pre-exponential factor of crude oil with noise

— real value; - - - estimated value of the first poles set; estimated value of the second poles set

Table 2 The mean errors of the catalyst circulation rate/kg·s⁻¹

Scenarios	Square signal		Sinusoidal signal	
	No noise	Noise	No noise	Noise
the first poles set	0.506	0.640	1.812	1.881
the second poles set	0.641	0.676	1.862	1.925

Table 3 The mean errors of the reaction rate constant pre-exponential factor/10⁻³ Pa⁻¹·s⁻¹

Scenarios	Square signal		Sinusoidal signal	
	No noise	Noise	No noise	Noise
the first poles set	0.693	0.794	1.833	1.967
the second poles set	1.201	1.232	3.141	3.160

error without noise and the more negative assigned poles also give less mean error. The modified model parameter is used for the online calculation of the state observer, effectively improving the robustness of the soft sensor.

6 CONCLUSIONS

For the nonlinear singular system in chemical processes, the unknown inputs and uncertain model parameters are augmented as state variables. On the basis of the observability of the singular system, a simplified observability criterion under certain conditions is presented for unknown input and uncertain model parameters. The augmented system will not be observable if the dimension of the unknown input plus the dimension of the uncertain model parameters is larger than the dimension of the measured output.

When the observability is satisfied, a soft sensor using augmented nonlinear singular state observer is used to estimate the unknown inputs and uncertain model parameters. For the FCCU riser reactor, with only the catalyst circulation rate unknown and no

uncertain model parameter, only one temperature sensor at the riser outlet can ensure that the catalyst circulation rate is correctly estimated by soft sensor. When an unknown input and an uncertain model parameter exist, however, another temperature sensor should be added to satisfy the necessary observability condition. Then the catalyst circulation rate and the uncertain model parameter can be estimated correctly by soft sensor.

NOMENCLATURE

A	systemic matrix of singular system
B	input matrix of singular system
C	output matrix of singular system
C_{ra}	coke mass percentage of catalyst in riser, %
E	singular matrix
E_A, E_φ	reaction activation energy of oil cracking and catalyst deactivation, kJ·kmol ⁻¹
e	observation error
F	unknown input matrix of singular system
F_O	flow rate of crude oil, kg·s ⁻¹
f	state equation
G	uncertain parameter matrix of singular system
G_C	catalyst circulation rate, kg·s ⁻¹
ΔH_{AA}	coke adsorption heat, kJ·kg ⁻¹
$\Delta H_{AR}, \Delta H_{DR}, \Delta H_{NR}$	cracking reaction heat of crude oil, diesel and gasoline, kJ·kg ⁻¹
h	output equation
K	state feedback gain matrix
k_{A0}, k_{D0}, k_{N0}	pre-exponential factor of reaction rate constant of crude oil, diesel and gasoline, Pa ⁻¹ ·s ⁻¹
$k_{\varphi0}$	pre-exponential factor of reaction rate constant of catalyst deactivation, Pa ⁻¹
L	output feedback matrix of state observer
l	dimension of outputs
m	dimension of inputs
N	number of riser segments
n	dimension of states
P, Q	equivalent transform matrix
p	uncertain model parameter
p_{ra}	pressure of riser reactor, Pa
q	rank of singular matrix

R	gas constant, $8.314 \text{ kJ} \cdot \text{kmol}^{-1} \cdot \text{K}^{-1}$
S_T	reaction time, s
T_{ra}	temperature of riser reactor, K
u	known control input
v	unknown input
x	state of singular system
y	measurable output
y_A, y_D, y_N, y_G	unconverted oil rate, diesel yield, gasoline yield, gas yield, % (by mass)
y_0	unmeasurable output
Γ	correction coefficient of heat capacity for tube
Λ	correction coefficient of heat capacity for oil
$\nu_{\text{AD}}, \nu_{\text{AN}}, \nu_{\text{AG}}, \nu_{\text{AC}}$	stoichiometric coefficient of oil-diesel reaction, oil-gasoline reaction, oil-gas reaction, oil-coke reaction
$\nu_{\text{DN}}, \nu_{\text{DG}}, \nu_{\text{DC}}, \nu_{\text{NG}}$	stoichiometric coefficient of diesel-gasoline reaction, diesel-gas reaction, diesel-coke reaction, gasoline-gas reaction
ϕ	activity of catalyst, %

Superscripts

—	the first equivalent form
~	the second equivalent form
^	estimated value
'	derivative of time

Subscripts

e	augmented system
0	primary variables
1	differential
2	algebraic

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APPENDIX

Proof of Theorem 2

Consider a linear singular system described by

$$\begin{cases} E\dot{x} = Ax + Bu \\ y = Cx \end{cases},$$

where $E \in \mathbf{R}^{n \times n}$ is singular, and $\text{rank}(E) = q < n$. $r = \text{degdet}(sE - A)$ is assumed, and obviously, $r \leq q < n$. (E, A) is said to be impulse-free if (E, A) is regular and $r = q$.

Lemma 3 [37] (E, A) is stable and impulse-free if and only if a matrix Y exists, such that

$$A^T Y + Y^T A < 0,$$

$$E^T Y = Y^T E \geq 0.$$

Theorem 2 $x = 0$ is assumed to be an equilibrium point

for the nonlinear singular system $E\dot{x} = f(x)$ and $A = \frac{\partial f}{\partial x} \Big|_{x=0}$,

where $f: D \rightarrow \mathbf{R}^n$ is continuously differentiable, and D is the neighbourhood near the origin. If (E, A) is stable and impulse-free, the nonlinear singular system $E\dot{x} = f(x)$ is asymptotically stable near the origin.

Proof The origin $x = 0$ is an equilibrium point for the nonlinear singular system [i.e., $f(0) = 0$]. The nonlinear system is linearized near the origin

$$f(x) = Ax + g(x).$$

As (E, A) is stable and impulse-free, $V(x) = x^T E^T Y x$ is used as the Lyapunov function for the nonlinear singular system. The

derivative of $V(x)$ of the system is given by

$$\begin{aligned} \dot{V}(x) &= (E\dot{x})^T Y x + x^T Y^T (E\dot{x}) \\ &= [Ax + g(x)]^T Y x + x^T Y^T [Ax + g(x)] \\ &= x^T [A^T Y + Y^T A] x + g^T(x) Y x + x^T Y^T g(x) \\ &= -x^T W x + 2(Yx)^T g(x) \end{aligned}$$

From **Lemma 3**, $W > 0$ can be derived. Thus, the first term on the right of the equation is negative.

Due to the continuous function, $g(x)$ satisfies

$$\frac{\|g(x)\|_2}{\|x\|_2} \rightarrow 0 \quad \text{as} \quad \|x\|_2 \rightarrow 0.$$

Therefore, for any $\gamma > 0$, an $r > 0$ exists, such that

$$\|g(x)\|_2 < \gamma \|x\|_2, \quad \forall \|x\|_2 < r.$$

Hence,

$$\begin{aligned} \dot{V}(x) &\leq -\lambda_{\min}(W) \|x\|_2^2 + 2\gamma \|Yx\|_2 \|x\|_2 \\ &\leq -\lambda_{\min}(W) \|x\|_2^2 + 2\gamma \|Y\|_2 \|x\|_2^2 \\ &= -[\lambda_{\min}(W) - 2\gamma \|Y\|_2] \|x\|_2^2, \quad \forall \|x\|_2 < r, \end{aligned}$$

where $\lambda_{\min}(\cdot)$ is the minimum eigenvalue of a matrix.

As W is symmetric and positive definite, $\lambda_{\min}(W)$ is real and positive. $\gamma < \frac{\lambda_{\min}(W)}{2\|Y\|_2}$, which ensures that $\dot{V}$ is negative

definite. Thus the nonlinear singular system $E\dot{x} = f(x)$ is asymptotically stable near the origin.

This procedure completes the proof.