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A COMPARISON OF DIFFERENT EKF APPROACHES FOR PARAMETERS ESTIMATION

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Abstract: In many chemical engineering applications the extended Kalman filter (EKF) is often used to deal with certain classes of nonlinear systems. This paper compares basic and polynomial approach of EKF for parameters estimation of nonlinear continuous-time stochastic systems. The proposed approaches are used to estimate constants k_{11} and k_{22} for interacting tank-in-series process and frequency factor k_0 and temperature of reaction mixture \mathcal{G} for continuous stirred-tank reactor (CSTR).

Keywords: Extended Kalman filter, nonlinear systems, parameter estimation, polynomial filtering

1 INTRODUCTION

Parameter estimation is one of the steps involved in the formulation and validation of a mathematical model and refers to the process of obtaining values of the parameters from the matching of the model-based calculated values to the set of measurements (data). (Englezos *et al.* 2001)

Many papers have studied parameters estimation using various techniques. In (Hernández-Barajas *et al.* 2009) comprehensive approach to estimate kinetic parameters when the involved reactions contain lumped chemical species is presented. This approach is based on representing rate constants with a continuous probability distribution function. In (Cheng 1996) simultaneously both heat transfer and kinetic parameters estimation under reacting conditions in a single tube wall-cooled fixed-bed reactor, and a two-stage parameter estimation was developed. The advantages of using maximum-likelihood estimators rather than simple least-squares estimators for the problem of finding unsaturated hydraulic parameters were demonstrated in (Hollenbeck *et al.* 1998). In (Esposito *et al.* 1998) global optimization approach tailored to the error-in-variables parameter estimation problem for nonlinear algebraic model was presented. A modified genetic algorithm to solve the

parameter identification problem for nonlinear digital filter was used in (Leehter *et al.* 1994). Model estimation using fast orthogonal search is presented in (Eklund *et al.* 2007).

In this work we apply basic and polynomial approaches of EKF to estimate constants k_{11} and k_{22} for interacting tank-in-series process and frequency factor k_0 and temperature of reaction mixture \mathcal{G} for continuous stirred-tank reactor and compare their performance.

2 THE CONTINUOUS-TIME EXTENDED KALMAN FILTER

Consider the following general nonlinear system model (Simon 2006):

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{w}, t) \\ \mathbf{y} &= \mathbf{h}(\mathbf{x}, \mathbf{v}, t) \\ \mathbf{w} &\sim (0, \mathbf{Q}) \\ \mathbf{v} &\sim (0, \mathbf{R})\end{aligned}\tag{1}$$

where $\mathbf{f}(\cdot)$ and $\mathbf{h}(\cdot)$ are general nonlinear functions. The noise processes \mathbf{w} and \mathbf{v} are white, zero-mean, uncorrelated, and have known covariance matrices \mathbf{Q} and \mathbf{R} . Equation (1) is expanded using Taylor series around a nominal control \mathbf{u}_0 , nominal state \mathbf{x}_0 , nomi-

nal output y_θ , and nominal noise values w_θ and v_θ . This gives the following approximately correct linear system

$$\begin{aligned}\Delta\dot{\mathbf{x}} &= A\Delta\mathbf{x} + L\mathbf{w} \\ &= A\Delta\mathbf{x} + \tilde{\mathbf{w}} \\ \tilde{\mathbf{w}} &\sim (0, \tilde{\mathbf{Q}}), \tilde{\mathbf{Q}} = L\mathbf{Q}L^T \\ \Delta\mathbf{y} &= C\Delta\mathbf{x} + M\mathbf{v} \\ &= C\Delta\mathbf{x} + \tilde{\mathbf{v}} \\ \tilde{\mathbf{v}} &\sim (0, \tilde{\mathbf{R}}), \tilde{\mathbf{R}} = M\mathbf{R}M^T\end{aligned}\quad (2)$$

The Δ quantities in the above equations are defined as deviations from the nominal trajectory:

$$\begin{aligned}\Delta\dot{\mathbf{x}} &= \dot{\mathbf{x}} - \dot{\mathbf{x}}_\theta \\ \Delta\mathbf{y} &= \mathbf{y} - \mathbf{y}_\theta\end{aligned}\quad (3)$$

where

$$\begin{aligned}\dot{\mathbf{x}}_\theta &= \mathbf{f}(\mathbf{x}_\theta, \mathbf{u}_\theta, \mathbf{w}_\theta, t) \\ \mathbf{y}_\theta &= \mathbf{h}(\mathbf{x}_\theta, \mathbf{v}_\theta, t)\end{aligned}\quad (4)$$

We assume that the control $\mathbf{u}(t)$ is perfectly known, so that $\mathbf{u}_\theta(t) = \mathbf{u}(t)$ and $\Delta\mathbf{u}(t) = \mathbf{0}$. The matrices on the right side of (2) are given as

$$\mathbf{A} = \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right|_\theta, \mathbf{L} = \left. \frac{\partial \mathbf{f}}{\partial \mathbf{w}} \right|_\theta, \mathbf{C} = \left. \frac{\partial \mathbf{h}}{\partial \mathbf{x}} \right|_\theta, \mathbf{M} = \left. \frac{\partial \mathbf{h}}{\partial \mathbf{v}} \right|_\theta \quad (5)$$

The Kalman filter equations for the linearized Kalman filter are

$$\begin{aligned}\Delta\dot{\hat{\mathbf{x}}} &= A\Delta\hat{\mathbf{x}} + \mathbf{K}(\Delta\mathbf{y} - C\Delta\hat{\mathbf{x}}) \\ \mathbf{K} &= \mathbf{P}\mathbf{C}^T \tilde{\mathbf{R}}^{-1} \\ \dot{\mathbf{P}} &= \mathbf{A}\mathbf{P} + \mathbf{P}\mathbf{A}^T + \tilde{\mathbf{Q}} - \mathbf{P}\mathbf{C}^T \tilde{\mathbf{R}}^{-1} \mathbf{C}\mathbf{P} \\ \hat{\mathbf{x}} &= \mathbf{x}_\theta + \Delta\hat{\mathbf{x}}\end{aligned}\quad (6)$$

where \mathbf{P} is equal to the covariance of the estimation error.

Now we will extend the linearized Kalman filter to directly estimate the states of a nonlinear system and linearize the nonlinear system around the Kalman filter estimate. This is the idea of EKF.

Combine the $\dot{\mathbf{x}}_\theta$ in equation (4) with $\Delta\dot{\hat{\mathbf{x}}}$ the expression in equation (6) to obtain

$$\begin{aligned}\dot{\mathbf{x}}_\theta + \Delta\dot{\hat{\mathbf{x}}} &= \mathbf{f}(\mathbf{x}_\theta, \mathbf{u}_\theta, \mathbf{w}_\theta, t) + A\Delta\hat{\mathbf{x}} + \\ &+ \mathbf{K}[\mathbf{y} - \mathbf{y}_\theta - C(\hat{\mathbf{x}} - \mathbf{x}_\theta)]\end{aligned}\quad (7)$$

Now choose $\mathbf{x}_\theta(t) = \hat{\mathbf{x}}(t)$ so that $\Delta\hat{\mathbf{x}}(t) = \mathbf{0}$ and $\Delta\dot{\hat{\mathbf{x}}}(t) = \mathbf{0}$. Then equation (7) becomes

$$\dot{\hat{\mathbf{x}}} = \mathbf{f}(\hat{\mathbf{x}}, \mathbf{u}, \mathbf{w}_\theta, t) + \mathbf{K}[\mathbf{y} - \mathbf{h}(\hat{\mathbf{x}}, \mathbf{v}_\theta, t)] \quad (8)$$

The continuous-time EKF can be summarized as follows:

Compute the following partial derivative matrices evaluated at the current state estimate:

$$\mathbf{A} = \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right|_{\hat{\mathbf{x}}}, \mathbf{L} = \left. \frac{\partial \mathbf{f}}{\partial \mathbf{w}} \right|_{\hat{\mathbf{x}}}, \mathbf{C} = \left. \frac{\partial \mathbf{h}}{\partial \mathbf{x}} \right|_{\hat{\mathbf{x}}}, \mathbf{M} = \left. \frac{\partial \mathbf{h}}{\partial \mathbf{v}} \right|_{\hat{\mathbf{x}}} \quad (9)$$

Compute the following matrices:

$$\begin{aligned}\tilde{\mathbf{Q}} &= L\mathbf{Q}L^T \\ \tilde{\mathbf{R}} &= M\mathbf{R}M^T\end{aligned}\quad (10)$$

Execute the following Kalman filter equations:

$$\begin{aligned}\dot{\hat{\mathbf{x}}} &= \mathbf{f}(\hat{\mathbf{x}}, \mathbf{u}, \mathbf{w}_\theta, t) + \mathbf{K}[\mathbf{y} - \mathbf{h}(\hat{\mathbf{x}}, \mathbf{v}_\theta, t)] \\ \mathbf{K} &= \mathbf{P}\mathbf{C}^T \tilde{\mathbf{R}}^{-1} \\ \dot{\mathbf{P}} &= \mathbf{A}\mathbf{P} + \mathbf{P}\mathbf{A}^T + \tilde{\mathbf{Q}} - \mathbf{P}\mathbf{C}^T \tilde{\mathbf{R}}^{-1} \mathbf{C}\mathbf{P}\end{aligned}\quad (11)$$

where the nominal noise values are given as $\mathbf{w}_\theta = \mathbf{0}$ and $\mathbf{v}_\theta = \mathbf{0}$.

This is the **basic approach of EKF** where Kalman gain matrix \mathbf{K} design is based on covariance matrix of estimation error \mathbf{P} obtained from differential Riccati equation.

Now we will derive the **polynomial approach of EKF**. Kalman gain matrix \mathbf{K} design is based on solution of the Diophantine equation.

Matrix transfer functions of the observable system (Mikleš *et al.* 2007) are given as

$$\mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1} = \mathbf{A}_L^{-1}(s)\mathbf{B}_{Ls}(s) \quad (12)$$

where $\mathbf{A}_L, \mathbf{B}_{Ls}$ are left coprime polynomial matrices and \mathbf{A}_L is row reduced.

If the gain matrix \mathbf{K} exist, it is unique and of the form

$$\mathbf{K} = \mathbf{Y}_R \mathbf{X}_R^{-1} \quad (13)$$

Then \mathbf{X}_R and \mathbf{Y}_R are solution of the Diophantine equation

$$\mathbf{A}_L(s)\mathbf{X}_R + \mathbf{B}_{Ls}(s)\mathbf{Y}_R = \mathbf{O}_L(s) \quad (14)$$

$\mathbf{O}_L(s)$ is a stable polynomial matrix with $\det \mathbf{O}_L(s) \neq 0$ and is given from spectral factorization as follows. Adding $s\mathbf{P}$ to either side of algebraic Riccati equation (assuming, that the noise processes have known covariance matrices \mathbf{Q} and $\mathbf{R} = \mathbf{I}$)

$$\mathbf{A}\mathbf{P} + \mathbf{P}\mathbf{A}^T - \mathbf{P}\mathbf{C}^T \mathbf{C}\mathbf{P} = -\mathbf{Q} \quad (15)$$

gives

$$(s\mathbf{I} - \mathbf{A})\mathbf{P} + \mathbf{P}(-s\mathbf{I} - \mathbf{A}^T) = \mathbf{Q} - \mathbf{P}\mathbf{C}^T \mathbf{C}\mathbf{P} \quad (16)$$

Multiplying from left by $\mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}$ and from right by $(-s\mathbf{I} - \mathbf{A}^T)^{-1} \mathbf{C}^T$ and using (11), (12) yields

$$\begin{aligned}\mathbf{A}_L(s)\mathbf{K}^T \mathbf{B}_{Ls}^T(s) + \mathbf{B}_{Ls}(s)\mathbf{K}\mathbf{A}_L^T(-s) + \\ + \mathbf{B}_{Ls}(s)\mathbf{K}\mathbf{K}^T \mathbf{B}_{Ls}^T(-s) = \mathbf{B}_{Ls}(s)\mathbf{Q}\mathbf{B}_{Ls}^T(-s)\end{aligned}\quad (17)$$

Adding $\mathbf{A}_L(s)\mathbf{A}_L^T(-s)$ to either side of this equation gives

$$\begin{aligned} (\mathbf{A}_L(s) + \mathbf{B}_{Ls}(s)\mathbf{K})(\mathbf{A}_L^T(-s) + \mathbf{K}^T \mathbf{B}_{Ls}^T(-s)) = \\ = \mathbf{A}_L(s)\mathbf{A}_L^T(-s) + \mathbf{B}_{Ls}(s)\mathbf{Q}\mathbf{B}_{Ls}^T(-s) \end{aligned} \quad (18)$$

Then matrix $\mathbf{O}_L(s)$ can be found from the spectral factorization equation

$$\begin{aligned} \mathbf{O}_L(s)\mathbf{O}_L^T(-s) = \mathbf{A}_L(s)\mathbf{A}_L^T(-s) + \\ + \mathbf{B}_{Ls}(s)\mathbf{Q}\mathbf{B}_{Ls}^T(-s) \end{aligned} \quad (19)$$

3 PARAMETER ESTIMATION

In order to estimate the parameters θ , we first augment the state with the parameters as extra states with no dynamics to obtain an augment state vector (Simon 2006):

$$\tilde{\mathbf{x}} = \begin{bmatrix} \mathbf{x} \\ \theta \end{bmatrix} \quad (20)$$

Our augment system model can be written as

$$\dot{\tilde{\mathbf{x}}} = \begin{bmatrix} \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{w}, t) \\ \theta \end{bmatrix} = \tilde{\mathbf{f}}(\tilde{\mathbf{x}}, \mathbf{u}, \mathbf{w}, t) \quad (21)$$

Note that $\tilde{\mathbf{f}}(\tilde{\mathbf{x}}, \mathbf{u}, \mathbf{w}, t)$ is a nonlinear function of the augmented state $\tilde{\mathbf{x}}$.

We can therefore use an extended Kalman filter to estimate $\tilde{\mathbf{x}}$.

4 MATHEMATICAL MODELLING

4.1 Interacting tank-in-series process

We consider (Mikleš *et al.* 2007) the interacting tank-in-series process shown in Fig. 1. The process input variable is the flow rate q_0 .

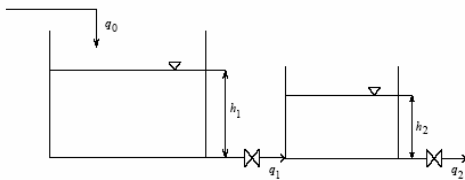


Fig. 1. An interacting tank-in-series process.

The process state variables are heights of liquid in tanks h_1, h_2 . Assuming that liquid density, F_1 and F_2 are constant, mass balance for the process yields

$$F_1 \frac{dh_1}{dt} = q_0 - q_1 \quad (22)$$

$$F_2 \frac{dh_2}{dt} = q_1 - q_2 \quad (23)$$

Inlet flow rate q_0 is independent of tank states whereas q_1 depends on the difference between liquid heights

$$q_1 = k_{11}\sqrt{h_1 - h_2} \quad (24)$$

Outlet flow rate q_2 depends on liquid height in the second tank

$$q_2 = k_{22}\sqrt{h_2} \quad (25)$$

Substituting q_1 from equation (24) and q_2 from (25) into (22) and (23) we get

$$\begin{aligned} \frac{dh_1}{dt} &= \frac{q_0}{F_1} - \frac{k_{11}}{F_1}\sqrt{h_1 - h_2} \\ \frac{dh_2}{dt} &= \frac{k_{11}}{F_2}\sqrt{h_1 - h_2} - \frac{k_{22}}{F_2}\sqrt{h_2} \end{aligned} \quad (26)$$

with arbitrary initial conditions

$$\begin{aligned} h_1(0) &= h_{10} \\ h_2(0) &= h_{20} \end{aligned} \quad (27)$$

To estimate constants k_{11} and k_{22} , two more equations are needed

$$\begin{aligned} \frac{dk_{11}}{dt} &= 0 & k_{11}(0) &= k_{11}^0 \\ \frac{dk_{22}}{dt} &= 0 & k_{22}(0) &= k_{22}^0 \end{aligned} \quad (28)$$

Equations (18) and (20) are now nonlinear system model for parameters estimation.

According to (9)

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (29)$$

where

$$\begin{aligned} a_{11} &= -\frac{\hat{k}_{11}}{2F_1\sqrt{\hat{h}_1 - \hat{h}_2}} & a_{12} &= \frac{\hat{k}_{11}}{2F_1\sqrt{\hat{h}_1 - \hat{h}_2}} \\ a_{13} &= -\frac{\sqrt{\hat{h}_1 - \hat{h}_2}}{F_1} & a_{21} &= \frac{\hat{k}_{11}}{2F_2\sqrt{\hat{h}_1 - \hat{h}_2}} \\ a_{22} &= -\frac{\hat{k}_{11}}{2F_2\sqrt{\hat{h}_1 - \hat{h}_2}} - \frac{\hat{k}_{22}}{2F_2\sqrt{\hat{h}_2}} \\ a_{23} &= \frac{\sqrt{\hat{h}_1 - \hat{h}_2}}{F_2} & a_{24} &= -\frac{\sqrt{\hat{h}_2}}{F_2} \end{aligned}$$

and

$$\mathbf{C} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad (30)$$

Parameters of the interacting tank-in-series process are shown on Table 1.

q_0	1	$\text{m}^3 \text{h}^{-1}$
k_{11}	0.8	$\text{m}^{5/2} \text{h}$
k_{22}	1.5	$\text{m}^{5/2} \text{h}$
F_1	0.8	m^2
F_2	0.8	m^2

Tab. 1. Parameters of the interacting tank-in-series process.

4.2 Continuous stirred-tank reactor

We consider CSTR (Mikleš *et al.* 2007) with a simple exothermal reaction $A \rightarrow B$ (Fig. 2.).

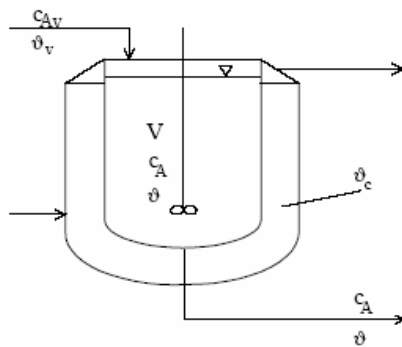


Fig. 2. A nonisothermal CSTR.

For the development of a mathematical model of the CSTR, the following assumptions are made: neglected heat capacity of inner walls of the reactor, constant density and specific heat capacity of liquid, constant reactor volume, constant overall heat transfer coefficient, and constant and equal input and output volumetric flow rates. As the reactor is well-mixed, the outlet stream concentration and temperature are identical with those in the tank.

A mass balance of component A can be expressed as

$$V \frac{dc_A}{dt} = qc_{AV} - qc_A - Vr(c_A, \vartheta) \quad (31)$$

The rate of reaction is strong function of concentration and temperature (Arrhenius law)

$$r(c_A, \vartheta) = kc_A = k_0 e^{-\frac{E}{R\vartheta}} c_A \quad (32)$$

Heat balance gives

$$V\rho c_P \frac{d\vartheta}{dt} = q\rho c_P \vartheta_v - q\rho c_P \vartheta - \alpha F(\vartheta - \vartheta_c) + V(-\Delta H)r(c_A, \vartheta) \quad (33)$$

Initial conditions are

$$\begin{aligned} c_A(0) &= c_{A0} \\ \vartheta(0) &= \vartheta_0 \end{aligned} \quad (34)$$

To estimate the temperature of reaction mixture ϑ and frequency factor k_0 , one more equation is needed

$$\frac{dk_0}{dt} = 0 \quad k_0(0) = k_0^0 \quad (35)$$

Equations (31), (33) and (35) are now nonlinear system model for parameters estimation.

According to (9)

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ 0 & 0 & 0 \end{pmatrix} \quad (36)$$

where

$$\begin{aligned} a_{11} &= -\frac{q}{V} - \hat{k}_0 e^{-\frac{g}{\vartheta}} & a_{12} &= -\frac{\hat{c}_A g \hat{k}_0 e^{-\frac{g}{\vartheta}}}{R \hat{\vartheta}^2} \\ a_{13} &= -\hat{c}_A e^{-\frac{g}{\vartheta}} & a_{21} &= \frac{\hat{k}_0 e^{-\frac{g}{\vartheta}} (-\Delta H) \hat{c}_A}{\rho c_P} \\ a_{22} &= -\frac{q}{V} - \frac{\alpha F}{V \rho c_P} + \frac{\hat{k}_0 g e^{-\frac{g}{\vartheta}} (-\Delta H) \hat{c}_A}{\hat{\vartheta}^2 \rho c_P} \\ a_{23} &= -\frac{e^{-\frac{g}{\vartheta}} (-\Delta H) \hat{c}_A}{\rho c_P} \end{aligned}$$

and

$$C = (1 \quad 0 \quad 0) \quad (37)$$

Parameters of the reaction and reactor are shown on Table 2.

c_{AV}	1.2	kmol m^{-3}
c_P	4.05	$\text{kJ kg}^{-1} \text{K}^{-1}$
E	107280	kJ kmol^{-1}
F	6.08	m^2
k_0	7.93e15	min^{-1}
V	1.7	m^3
ΔH	-150000	kJ kmol^{-1}
q	0.2	$\text{m}^3 \text{min}^{-1}$
R	8.314	$\text{kJ kmol}^{-1} \text{K}^{-1}$
α	41.2	$\text{kJ m}^{-2} \text{min}^{-1} \text{K}^{-1}$
ϑ_c	318	K
ϑ_v	313	K
ρ	998	kg m^{-3}

Tab. 2. Parameters of the reaction and reactor.

4 SIMULATION RESULTS

For the tank-in-series process parameters estimation simulation, the following values were tracked: $q_0(t) = 1 \text{ m}^3 \cdot \text{h}^{-1}$ for $t < 0 \text{ h}$ and $q_0(t) = 1.1 \text{ m}^3 \cdot \text{h}^{-1}$ for $t \geq 0 \text{ h}$. Initial condition for estimated parameters: $k_{11} = 1 \text{ m}^{5/2} \cdot \text{h}$, $k_{22} = 1 \text{ m}^{5/2} \cdot \text{h}$. True values of parameters are: $k_{11} = 0.8 \text{ m}^{5/2} \cdot \text{h}$ and $k_{22} = 1.5 \text{ m}^{5/2} \cdot \text{h}$. Fig. 3,4 show the estimation results for tank-in-series process.

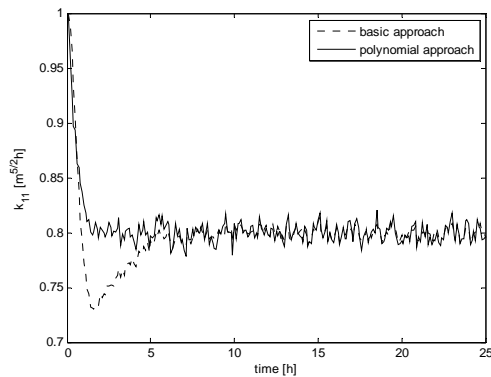


Fig. 3. Estimation of the k_{11} constant.

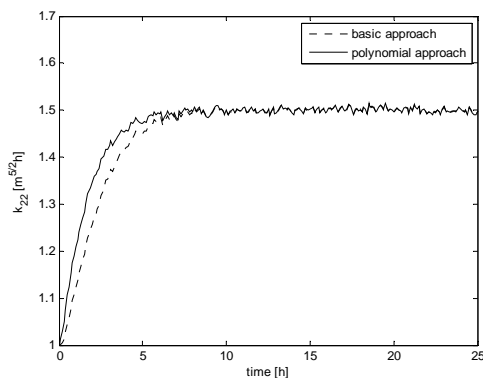


Fig. 4. Estimation of the k_{22} constant.

For the CSTR parameters estimation simulation, the following values were tracked: $c_{A0}(t) = 1.2 \text{ kmol} \cdot \text{m}^{-3}$ for $t < 0 \text{ h}$ and $c_{A0}(t) = 1.15 \text{ kmol} \cdot \text{m}^{-3}$ for $t \geq 0 \text{ h}$. Initial condition for estimated parameters: $\mathcal{G} = 320 \text{ K}$, $k_0 = 7 \times 10^{14} \text{ min}^{-1}$. Fig. 5,6 show the estimation results for CSTR. True value of parameter k_0 is $7.93 \times 10^{15} \text{ min}^{-1}$.

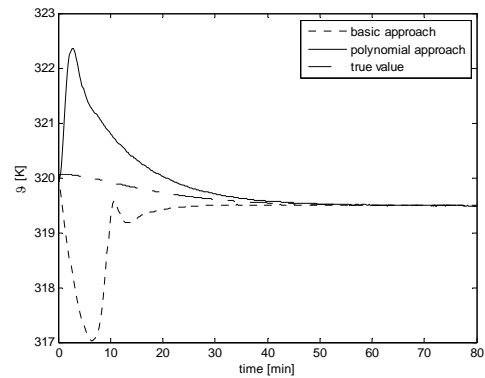


Fig. 5. Estimation of the temperature of reaction mixture \mathcal{G} .

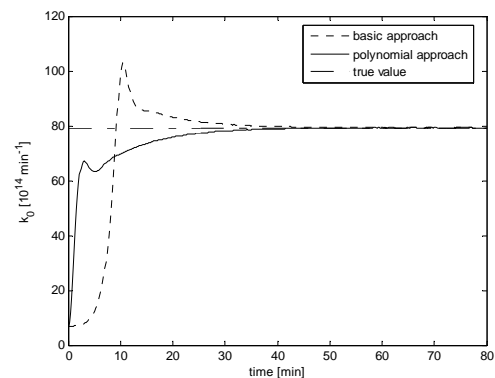


Fig. 6. Estimation of the frequency factor k_0 .

The estimation of parameters and states is carried out in presence of noise. Because there is no general rule for the choice of the matrix \mathbf{Q} , it was chosen experimentally in order to ensure its positive definition (diagonal matrix). From the results it is observed that both presented approaches give very high accuracy of parameters estimation. But we can see that the performance of polynomial approach algorithm is higher than the performance of basic approach algorithm, because the true values of parameters are reached faster.

5 CONCLUSION

In this paper, parameters estimation of nonlinear continuous-time stochastic system using continuous-time extended Kalman filter (EKF) is presented. Basic and polynomial approach of Kalman gain matrix \mathbf{K} design was used to estimate constant k_{11} and k_{22} for interacting tank-in-series process and frequency factor k_0 and temperature of reaction mixture \mathcal{G} for continuous stirred-tank reactor.

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