A New Process Noise Covariance Matrix Tuning Algorithm for Kalman Based State Estimators

Nina P. G. Salau*, Jorge O. Trierweiler*, Argimiro R. Secchi**, Wolfgang Marquardt***

 * Federal University of Rio Grande do Sul, Chemical Engineering Department, Eng. Luiz Englert, s/n°, Campus Central, CEP 90040-040, Porto Alegre - RS, Brazil, (ninas@ enq.ufrgs.br, jorge@ enq.ufrgs.br)
 ** Federal University of Rio de Janeiro, PEQ – COPPE, Av. Horácio Macedo, 2030 - Centro de Tecnologia - Bloco G - Sala G-115, Cidade Universitária, CP: 68502, CEP 21945-970, Rio de Janeiro – RJ, (arge@ peq.coppe.ufrj.br)
 **RWTH Aachen University, Process Systems Engineering,Turmstr. 46, 52064 Aachen, Germany, (wolfgang.marquardt@avt.rwth-aachen.de)

Abstract: A suitable design of state estimators requires a representative model for capturing the plant behavior and knowledge about the noise statistics, which are generally not known in practical applications. While the measurement noise covariance can be directly derived from the measurement device reproducibility, the choice of the process noise covariance is much less straightforward. Further, processes such as continuous process with grade transitions and batch or semi-batch process are characterized by time-varying structural uncertainties which are, in many cases, partially and indirectly reflected in the uncertainty of the model parameters. It has been shown that the robust performance of state estimators significantly enhances with a time-varying and non-diagonal process noise covariance matrix, which explicitly takes parameter uncertainty into account. For this case, the parameter uncertainty is quantified through the parameter covariance matrix. This paper presents a direct and a sensitivity method for the parameter covariance matrix computation. In the direct method, the parameter covariance matrix is obtained through a time-varying sensitivity matrix. The results have shown the efficacy of these methods in improving the performance of an extended Kalman filter (EKF) for a semi-batch reactor process.

Keywords: state estimator design, noise statistics, parameter estimation, sensitivity analyses.

1. INTRODUCTION

Since usually not all states of a nonlinear dynamic model are measured, they need to be estimated to be used in any control and optimization strategy. State estimators are used to estimate the unmeasured states and to filter the measured ones. Therefore, they are essential for any advanced control and optimization application. Besides an accurate plant model, an appropriate choice of process and measurement noise covariances is crucial in applying state estimators. The measurement error covariance matrix is usually known from the error statistics of the measurement device and is readily available. However, in actual problems, the process-noise statistics are often unknown, do not satisfy the assumptions of normal distribution and are mostly due to the uncertainties in the model that can be either parametric or structural.

Adaptive filtering techniques estimate noise covariances from data and have been used for nonlinear systems (Mehra, 1972; Odelson et al. 2006). The methods in this field can be divided into four general categories (Mehra, 1972): Bayesian, maximum likelihood, covariance matching, and correlation techniques. Bayesian and maximum likelihood methods have fallen out of favor because of their sometimes excessive computation times. Covariance matching is the computation of the covariances from the residuals of the state estimation problem, but has been shown to give biased estimates of the true covariances. The fourth category is correlation techniques, which is the most popular for determining these covariances (Odelson et al. 2006). However, these methods assume constant noise characteristics and the availability of data required to obtain a true representation of noise statistics. For continuous or batch processes with timevarying process dynamics and operating within a wide range of process conditions, these noise statistics are time varying. The use of a fixed value of noise statistics can lead to poor filter performance and even result in filter divergence (Vallapil & Georgakis 1999, 2000, Leu & Baratti, 2000).

Valappil & Georgakis (1999, 2000) introduced two systematic approaches to be used for the calculation of a time-varying and non-diagonal process noise covariance matrix, which explicitly takes parameter uncertainty into account. The first, called linearized approach, is based on a Taylor series expansion of the nonlinear equations around the nominal parameter values, while the second, called Monte Carlo approach, accounts for the nonlinear dependence of the system on the fitted parameters by Monte Carlo simulations that can easily be performed on-line. Both approaches have been compared favorably with the traditional methods of trial-and-error tuning of EKF. For the linearized approach, the process noise covariance matrix for the filter is obtained by a procedure using the known parameter covariance matrix. The main advantage of the linearized approach is that it involves very simple algebraic calculations and can easily be executed on-line. Afterwards this approach was employed successfully in EKF-based NMPC algorithms for batch

processes (Valappil & Georgakis, 2001, 2002; Nagy and Braatz, 2003).

In this work, a new process noise covariance matrix tuning algorithm is proposed. It is an extension of the linearized approach proposed by Valappil and Georgakis (1999, 2000) with two methods for the parameter covariance matrix computation. In the direct method, the parameter covariance matrix is found during the parameter estimation step using SELEST (Secchi et al., 2006), an algorithm for automatic selection of model parameters based on an extension of the identifiability measure of Li et al. (2004). In the sensitivity method, the parameter covariance matrix is obtained through a time-varying sensitivity matrix. Both methods can be successfully applied for state estimator design.

2. PROBLEM FORMULATION AND SOLUTION STRATEGIES

2.1 Hybrid Extended Kalman Filter (H-EKF)

Consider the following nonlinear dynamic system to be used in the state estimator

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{t}, \mathbf{p}) + \boldsymbol{\omega}(\mathbf{t})$$

$$\mathbf{y}_{\mathbf{k}} = \mathbf{h}_{\mathbf{k}}(\mathbf{x}_{\mathbf{k}}, \mathbf{t}_{\mathbf{k}}) + \boldsymbol{\nu}_{\mathbf{k}}$$

$$\boldsymbol{\omega}(\mathbf{t}) \sim (\mathbf{0}, \mathbf{Q}) \qquad (1)$$

$$\boldsymbol{\nu}_{\mathbf{k}} \sim (\mathbf{0}, \mathbf{R}_{\mathbf{k}})$$

where u denotes the deterministic inputs, x denotes the states, and y denotes the measurements. The process-noise vector, $\omega(t)$, and the measurement-noise vector, v_k , are assumed to be a white Gaussian random process with zero mean and covariance Q and R_k, respectively. The H-EKF formulation uses a continuous and nonlinear model for state estimation, linearized models of the nonlinear system for state covariance estimation, and discrete measurements (Simon, 2006). This is often referred to as continuous-discrete extended Kalman filter (Jazwinski, 1970). Here, the system is linearized at each time step to obtain the local state-space matrices as below:

$$F(t) = \left(\frac{\partial f}{\partial x}\right)_{x,u,t,p_{nom}}, \quad H(t) = \left(\frac{\partial h}{\partial x}\right)_{x,u,t,p_{nom}}$$
(2)

The equations that compose the different steps in the H-EKF are given below.

State transition equation:

$$\hat{x}_{k|k-1} = \hat{x}_{k-1|k-1} + \int_{k-1}^{k} f(\hat{x}, u, \tau, p) d\tau$$
(3)

State covariance transition equation

$$P_{k|k-1} = P_{k-1|k-1} + \int_{k-1}^{k} \left[F(\tau)P(\tau) + P(\tau)F(\tau)^{T} + Q \right] d\tau \qquad (4)$$

Kalman gain equation:

$$K_{k} = P_{k|k-1} H_{k}^{T} \left[H_{k} P_{k|k-1} H_{k}^{T} + R_{k} \right]^{-1}$$
(5)

State update equation:

$$\hat{\mathbf{x}}_{k|k} = \hat{\mathbf{x}}_{k|k-1} + \mathbf{K}_{k} \left[\mathbf{y}_{k} - \mathbf{h} \left(\hat{\mathbf{x}}_{k|k-1}, \mathbf{t}_{k} \right) \right]$$
 (6)

State covariance update equation:

$$\mathbf{P}_{\mathbf{k}|\mathbf{k}} = \left[\mathbf{I}_{\mathbf{n}} - \mathbf{K}_{\mathbf{k}} \mathbf{H}_{\mathbf{k}}\right] \mathbf{P}_{\mathbf{k}|\mathbf{k}-1} \left[\mathbf{I}_{\mathbf{n}} - \mathbf{K}_{\mathbf{k}} \mathbf{H}_{\mathbf{k}}\right]^{\mathrm{T}} + \mathbf{K}_{\mathbf{k}} \mathbf{R}_{\mathbf{k}} \mathbf{K}_{\mathbf{k}}^{\mathrm{T}}$$
(7)

2.2 Linearized Approach to Calculate the $\omega(t)$ Statistics

As introduced by Valappil & Georgakis (1999, 2000), the linearized approach to calculate the $\omega(t)$ statistics of (1) consists in assuming that the process noise vector $\omega(t)$ mostly represents the effects of parametric uncertainty. As $\dot{x}(t)$ and

 $\dot{x}_{nom}(t)$ are desired to be the same, $\omega(t)$ can be defined by

$$\omega(t) = f(x, u, t, p) - f(x_{nom}, u, t, p_{nom})$$
(8)

Performing a first-order Taylor's series expansion of the right-hand side of (8) around the nominal state trajectory (x_{nom}) and the nominal parameters (p_{nom}) , neglecting the higher-order terms, results in following approximation

$$\omega(t) = \left(\frac{\partial f}{\partial x}\right)_{x_{\text{nom}},u,t,p_{\text{nom}}} \left[x(t) - x_{\text{nom}}(t)\right] + \left(\frac{\partial f}{\partial p}\right)_{x_{\text{nom}},u,t,p_{\text{nom}}} \left[p - p_{\text{nom}}\right]$$
(9)

Assuming that $[x(t)-x_{nom}(t)] = [\hat{x}(t)-x_{nom}(t)] \approx 0$, the process noise is calculated from

$$\omega(t) = F_{P_{\text{nom}}}(t) [p - p_{\text{nom}}]$$
(10)

where $F_{p_{nom}}(t) = \left(\frac{\partial f}{\partial p}\right)_{\hat{x},u,t,p_{nom}}$. Calculating the expected

value of both sides of (10) yields

$$\overline{\omega}(t) = F_{p_{\text{nom}}}(t)(p_{\text{nom}} - p_{\text{nom}}) = 0$$
(11)

indicating that the noise sequence $\omega(t)$ has zero mean if the employed linearization in the parameters was accurate. Then the desired computation of the covariance Q(t) of $\omega(t)$ is given by

$$Q(t) = F_{P_{nom}}(t) C_{p} F_{P_{nom}}^{T}(t)$$
(12)

where $C_p \in \Re^{n_p \times n_p}$ is the parameter covariance matrix. In this work, we propose two methods to calculate C_p , which are presented in the next subsection.

2.3 Proposed Methods to Calculate the C_p Matrix

Consider the general process model.

$$\dot{\mathbf{x}} = \mathbf{f} \left(\mathbf{x}, \mathbf{u}, \mathbf{t}, \mathbf{p}_{\text{nom}} \right) \tag{13}$$

Differentiating (13) with respect to the nominal parameter vector, p_{nom} , gives

$$\dot{\mathbf{S}} = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right) \mathbf{S} + \left(\frac{\partial \mathbf{f}}{\partial \mathbf{p}_{\text{nom}}}\right) = \mathbf{F}(\mathbf{t}) \mathbf{S} + \mathbf{F}_{\mathbf{p}_{\text{nom}}}(\mathbf{t})$$
(14)

where S is the sensitivity matrix $(\partial x / \partial p_{nom})$ determined by numerical integration of (14) along with the model of (13).

2.3.1 Direct Method: Parameter Covariance Matrix via Parameter Estimation

In this method, C_p is constant and directly obtained from the parameter estimation procedure. For this purpose, we have selected the SELEST algorithm proposed by Secchi et al. (2006). This algorithm uses a sensitivity matrix, S, based on calculation of the parameters effects on the measured outputs and of a linear-independence metric, as proposed by Li et al. (2004). A predictability degradation index and a parameter correlation degradation index are used as stopping criterion. The definitions of these indexes as well as the SELEST algorithm are presented in Secchi et al. (2006).

2.3.2 Sensitivity Method: Parameter Covariance Matrix via Sensitivity Matrix

As pointed out by Sharma & Arora (1993), the sensitivity matrix, S, can play a role in quantifying how good the estimate of the parameters is. For uncorrelated and normally distributed measurement errors and for nonlinear least-squares problems, a parameter covariance matrix C_p can be estimated from

$$C_{p} \approx s^{2} \left(S^{T} S \right)^{-1}$$
(15)

where s^2 accounts for the accuracy of the data used to fit the parameters (\hat{Y}) and is usually represented by the residual mean square

$$s^{2} = \frac{\sum \left(\hat{Y} - Y_{p}\right)^{T} \left(\hat{Y} - Y_{p}\right)}{n - np}$$
(16)

where Y_p is the estimated data, n is the number of samples and np is the number of estimated parameters. The residual mean square s² is also obtained from the parameter estimation using SELEST algorithm. Since the sensitivity matrix, S, is time-varying, C_p is also time-varying, which represents an advantage of this method.

3. MATRIX Q TUNING ALGORITHM

This section presents an algorithm for tuning of the process noise covariance matrix. As mentioned earlier, this algorithm is an extension of the linearized approach proposed by Valappil and Georgakis (1999, 2000) with two methods for the parameter covariance matrix computation.

Since any model is an abstraction of reality, both the structural and parametric uncertainties are present to some degree in most real situations. The structural uncertainties is often captured by uncertainty in the model parameters only. The proposed algorithm requires knowledge about which parameters can be considered time-varying. Afterwards, SELEST algorithm estimates the best possible subset of parameters within a full set of model parameters assumed time-varying.

Parameter estimation is a key ingredient to quantify the parametric model uncertainty. However, most contributions on parameter estimation in process control assume that all model states are measured, which is not true in practical applications. In order to carry out proper parameter estimation, the EKF is used in a previous stage with the nominal parameters to estimate the unmeasured states and to filter the measured ones. Afterwards, the state estimation is carried out a posteriori with the estimated parameters, p_{est} , and a time-varying and non-diagonal matrix Q obtained from the procedure described above. The required covariance matrix C_p is calculated by one of the two methods proposed in this work. The structure of the algorithm for process noise covariance matrix Q tuning is shown in Fig. 1.



Fig. 1: Process noise covariance matrix Q tuning algorithm.

Note that the matrix Q in our algorithm takes into account the estimated parameters, p_{est} , rather than the nominal parameters, p_{nom} , as introduced by Vallapil and Georgakis (1999, 2000) in (12).

4. CASE STUDY: WILLIAMS-OTTO SEMI-BATCH REACTOR

A description of the Williams-Otto semi-batch reactor, as introduced by Forbes (1994), is provided in this section. The following reactions take place in the reactor:

$$A + B \xrightarrow{k_1} C$$

$$C + B \xrightarrow{k_2} P + E$$

$$P + C \xrightarrow{k_3} G$$

Reactant A is already present in the reactor, whereas reactant B is fed continuously to the reactor. During the exothermic reactions the products P and E as well the side-product G are formed. The heat generated through the exothermic reaction is removed by a cooling jacket, which is controlled by manipulating the cooling water temperature. The manipulated control variables of this process are the inlet flow rate of reactant B (F_B) and the cooling water temperature (T_w), whose values have been kept constant in our study. The model equations are given below and the model parameters are reported in Table 1:

$$\frac{\mathrm{dm}_{\mathrm{A}}}{\mathrm{dt}} = -\frac{\mathrm{M}_{\mathrm{A}}}{\mathrm{M}_{\mathrm{A}}} r_{\mathrm{l}} \mathrm{V} \tag{17}$$

$$\frac{\mathrm{d}m_{\mathrm{B}}}{\mathrm{d}t} = \mathrm{F}_{\mathrm{B}} - \frac{\mathrm{M}_{\mathrm{B}}}{\mathrm{M}_{\mathrm{A}}} \mathrm{r}_{\mathrm{I}} \mathrm{V} + \frac{\mathrm{M}_{\mathrm{B}}}{\mathrm{M}_{\mathrm{B}}} \mathrm{r}_{\mathrm{2}} \mathrm{V}$$
(18)

$$\frac{dm_{\rm C}}{dt} = \frac{M_{\rm C}}{M_{\rm A}} r_{\rm l} V - \frac{M_{\rm C}}{M_{\rm B}} r_{\rm 2} V - \frac{M_{\rm C}}{M_{\rm C}} r_{\rm 3} V$$
(19)

$$\frac{\mathrm{dm}_{\mathrm{P}}}{\mathrm{dt}} = \frac{\mathrm{M}_{\mathrm{P}}}{\mathrm{M}_{\mathrm{B}}} r_{2} \mathrm{V} - \frac{\mathrm{M}_{\mathrm{P}}}{\mathrm{M}_{\mathrm{C}}} r_{3} \mathrm{V} \tag{20}$$

$$\frac{\mathrm{dm}_{\mathrm{E}}}{\mathrm{dt}} = \frac{\mathrm{M}_{\mathrm{E}}}{\mathrm{M}_{\mathrm{B}}} r_{2} \mathrm{V} \tag{21}$$

$$\frac{\mathrm{dm}_{\mathrm{G}}}{\mathrm{dt}} = \frac{\mathrm{M}_{\mathrm{G}}}{\mathrm{M}_{\mathrm{C}}} \mathbf{r}_{\mathrm{3}} \mathbf{V} \tag{22}$$

$$\frac{\mathrm{dV}}{\mathrm{dt}} = \frac{\mathrm{F}_{\mathrm{B}}}{\mathrm{\rho}} \tag{23}$$

$$\frac{\mathrm{d}\mathrm{T}_{\mathrm{r}}}{\mathrm{d}\mathrm{t}} = \frac{\mathrm{H} - \mathrm{F}_{\mathrm{B}}\mathrm{c}_{\mathrm{p}}\mathrm{T}_{\mathrm{r}}}{\mathrm{V}\rho\,\mathrm{c}_{\mathrm{p}}}$$
(24)

where

$$V = \frac{m_{A} + m_{B} + m_{C} + m_{P} + m_{E} + m_{G}}{\rho}$$
(25)

$$r_1 = k_1 \frac{m_A m_B}{V^2}; \quad r_2 = k_2 \frac{m_B m_C}{V^2}; \quad r_3 = k_3 \frac{m_C m_P}{V^2}$$
 (26)

$$k_i = A_i e^{\overline{(T_r + T_{ref})}}; \quad i = 1, 2, 3$$
 (27)

$$H = F_{B}c_{p}T_{in} - \Delta H_{1}\frac{M_{A}}{M_{A}}r_{1}V - \Delta H_{2}\frac{M_{B}}{M_{B}}r_{2}V -\Delta H_{3}\frac{M_{C}}{M_{C}}r_{3}V - V\frac{A_{0}}{V_{0}}U(T_{r} - T_{w})$$
(28)

Table 1. Model Parameters

MA	100 kg.kmol ⁻¹	ΔH_1	-263.8 kJ.kg ⁻¹
M _B	200 kg.kmol ⁻¹	ΔH_2	-158.3 kJ.kg ⁻¹
M _C	200 kg.kmol ⁻¹	ΔH_3	-226.3 kJ.kg ⁻¹
M _P	100 kg.kmol ⁻¹	A_0	9.2903 m ²
M _E	200 kg.kmol ⁻¹	V_0	2.1052 m^3
M _G	300 kg.kmol ⁻¹	U	$0.23082 \text{ kJ}(\text{m}^2.^{\circ}\text{C.s})^{-1}$
A ₁	1.6599E3 m ³ kg ⁻¹ s ⁻¹	F _B	5.7840 kg.s ⁻¹
A ₂	7.2117E5 m ³ kg ⁻¹ s ⁻¹	T _w	100 °C
A ₃	2.6745E9 m ³ kg ⁻¹ s ⁻¹	$m_A(t_0)$	2000 kg
E ₁	6666.7 K	$m_B(t_0)$	0
E ₂	8333.3 K	$m_{\rm C}(t_0)$	0
E ₃	11111.1 K	$m_P(t_0)$	0
T _{ref}	273.15 K	$m_E(t_0)$	0
T _{in}	35 °C	$m_G(t_0)$	0
C _p	4.184 kJ.kg ⁻¹ .°C ⁻¹	$V(t_0)$	2 m^3
ρ	1000 kg.m ⁻³	$T_r(t_0)$	65 °C
t _f	1000 s		

In order to illustrate the application of the Q tuning algorithm, the kinetic parameters E_1 , E_2 , and E_3 were chosen as uncertain parameters. A parametric uncertainty of $\pm 5\%$ is assumed. The correct parameter values ("plant parameters"), p, and the nominal parameters, p_{nom} , are reported in Table 2.

Table 2. Uncertain Parameters

	E ₁	E ₂	E ₃
р	6333.4	7916.3	11666.6
p _{nom}	6666.7	8333.3	11111.1

The application of Q tuning algorithm to the Williams-Otto semi-batch reactor is shown below.

4.1 First Iteration of Q Tuning Algorithm.

4.1.1 Results of State Estimation: First Stage

A first state estimation with nominal parameters is performed to provide information on unmeasured states to be used in the subsequent parameter estimation step. The states and measurements of the Williams-Otto semi-batch reactor are

$$y = [m_B \quad m_E \quad m_G \quad V] \tag{30}$$

The measurements are obtained from a simulation of the plant model with the plant parameters p. The initial condition and the parameters of the state estimation are

$$\mathbf{x}_0 = \begin{bmatrix} 2000 & 0 & 0 & 0 & 0 & 2 & 65 \end{bmatrix}$$
(31)

$$P_0 = 0.0001^2 I_{8x8} \tag{32}$$

$$\Delta t = t_k - t_{k-1} = 31.25 \tag{33}$$

$$R = diag \begin{pmatrix} 0.1^2 & 0.1^2 & 0.01^2 & 0.01^2 \end{pmatrix}$$
(34)

$$Q=diag(0.1^{2} \quad 0.01^{2} \quad 0.1^{2} \quad 0.01^{2} \quad 0.01^{2} \quad 0.1^{2} \quad 0.1^{2} \quad 0.1^{2} \quad 0.01^{2}) (35)$$

The state estimation results using the EKF with nominal parameters and a constant-value and diagonal matrix Q are shown in Fig. 2. As expected, in the presence of a constant parametric model mismatch, the estimated states show a bias (cf. Fig. 2b).



Fig. 2: EKF with nominal parameters (pnom) and a constantvalue and diagonal matrix Q (Q_d): (a) filtered measured states and (b) estimated states.

4.1.2 Results of Parameter Estimation Step

Using the SELEST algorithm, the parameter estimation step is based on the nominal parameters, p_{nom} . The data used to fit the parameters are composed of the estimated states and the filtered measured states provided by the first state estimation stage. As a result of the parameter estimation step, the SELEST algorithm provides the estimated parameters, p_{est} , the parameter covariance matrix, C_p , and the residual mean square, s^2

$$p_{est} = \begin{bmatrix} 6333.8 & 7957.9 & 11223.5 \end{bmatrix}$$

$$C_{p} = \begin{bmatrix} 3.2469E - 5 & -8.6175E - 6 & -4.2417E - 5 \\ -8.6175E - 6 & 3.8060E - 5 & 8.2221E - 6 \\ -4.2417E - 5 & 8.2221E - 6 & 3.8060E - 5 \end{bmatrix}$$

$$s^{2} = \frac{\sum (\hat{Y} - Y_{p})^{T} (\hat{Y} - Y_{p})}{\left(\frac{t_{f}}{\Delta t} + 1\right) - np} = \frac{\sum (\hat{Y} - Y_{p})^{T} (\hat{Y} - Y_{p})}{\left(\frac{1000}{31.25} + 1\right) - 3} = 1.66E2$$

where \hat{Y} is composed of the estimated and the filtered measured states resulting from the first state estimation stage and Y_p is calculated by the SELEST algorithm.

4.1.3 Results of State Estimation: Second Stage

At this point, state estimation is carried out with the estimated parameters and the time-varying and non-diagonal Q obtained by C_p . The performance of the EKF with the following choices for calculating Q is compared and the results are shown in Fig. 3.

<u>Direct method</u>: Q is time-varying and non-diagonal, with p_{est} and C_p estimated by means of the SELEST algorithm.

<u>Sensitivity method</u>: Q is time-varying and non-diagonal, with p_{est} and s^2 estimated by means the SELEST algorithm and C_p obtained via sensitivity integration.

<u>Random Variation</u>: Proposed by Valappil and Georgakis (1999, 2000). The parameters in the plant are assumed to vary with time, taking values at each sample interval from a nominal distribution. The mean value of the varying plant parameter is assumed to be different from the nominal value of the model parameter by a fixed amount σ . The parameter covariance matrix used in the filter is given by $C_p = \sigma^2$.

<u>Monte Carlo Approach</u>: Proposed by Valappil and Georgakis (1999, 2000). This approach accounts for the nonlinear dependence of the system on the fitted parameters by Monte Carlo simulations. For the case study, 500 Monte Carlo simulations of different parameter values were used, resulting in 500 evaluations of the process noise.

The initial conditions (31) and the parameters of the state estimation algorithm (32 to 35) remain the same in this stage. According to Fig. 3, the EKF with a time-varying and nondiagonal matrix Q obtained by random variation in the plant parameters presents the worst performance. The sensitivity method performs better compared to the direct method. As mentioned before, an advantage of this method is that the parameter covariance matrix, C_p , is time-varying due to the time-varying sensitivity matrix S. In spite of accounting the nonlinear dependence of the system on the fitted parameters, the Monte Carlo shows a performance slightly inferior to the that of the sensitivity method for estimated states (Fig. 3b) and a performance quite inferior to that of the sensitivity and direct methods for measured states (Fig. 3a), not to mention the high computational effort.



Fig. 3: EKF with estimated parameters (p_{est}) and a timevarying and non-diagonal Q matrix obtained by the proposed methods: direct (Q_{dm}) and the sensitivity (Q_{sm}) ; and by the literature methods: random variation (Q_{rv}) and Monte Carlo (Q_{MC}) : (a) filtered measured states and (b) estimated states.

4.2 Second Iteration of Matrix Q Tuning Algorithm

Since the unmeasured states are unknown in practical applications, the state estimation accuracy shall be quantified. The matrix Q tuning algorithm is hence performed iteratively with the proposed methods for the parameter covariance matrix computation until the state estimation accuracy could not be significantly improved.

The parameter estimation is now taking place with the estimated parameters, p_{est} , and the estimated states and filtered measurements from the first iteration of the proposed algorithm. The parameter estimation results for both methods are given in Table 3.

Table 3. Uncertain Parameters

Mathad	p _{est}			°2
Method	E ₁	E ₂	E ₃	S
Direct	6328.1	7952.7	11668.9	7.0880
Sensitivity	6333.9	7921.3	11666.3	0.7785

Disregarding numerical round off, the matrix C_p is the same for both methods, i.e.

$$C_{p} = \begin{bmatrix} 4.9337E - 5 & -4.6902E - 6 & 4.3956E - 6 \\ -4.6902E - 5 & 7.7390E - 5 & 4.7829E - 6 \\ 4.3956E - 5 & 4.7829E - 6 & 5.0158E - 5 \end{bmatrix}$$

As expected, the residual mean square s^2 is smaller for the sensitivity method which performs better than direct method in an a-posteriori state estimation stage, as shown in Fig. 4.



Fig. 4: Estimated states for the EKF with estimated parameters (p_{est}) and a time-varying and non-diagonal Q matrix obtained by the direct (Q_{dm}) and the sensitivity (Q_{sm}) methods.

For this example, a third iteration of the algorithm has not improved significantly the state estimation accuracy.

5. CONCLUSIONS

A new process noise covariance matrix tuning algorithm is presented which incorporates the linearized approach proposed by Valappil and Georgakis (1999, 2000) with two methods for the parameter covariance matrix computation. As pointed out by Valappil and Georgakis (1999, 2000), the investment in a nondiagonal time-varying matrix Q is justified because (a) parametric uncertainties cause significant cross-correlations between the process noises for different states (b) for continuous or batch processes with time-varying process dynamics and operating on wide range of process conditions, the noise statistics are time varying.

The Q tuning algorithm consists of two state estimation steps and a parameter estimation step in between. A first state estimation step with nominal parameters is performed to provide information on unmeasured states to be used in the subsequent parameter estimation step. Afterwards, the state estimation is carried out with the estimated parameters and a time-varying and non-diagonal tuning of matrix Q obtained from the parameter covariance matrix C_p , evaluated by the direct and sensitivity methods. In the direct method, C_p is assumed to be constant and directly obtained from the parameter estimation step using the SELEST algorithm (Secchi et al., 2006). In the sensitivity method, C_p is obtained from the computation of the time-varying sensitivity matrix. Although the EKF with a time-varying and non-diagonal matrix Q obtained from the sensitivity method performs better compared to the direct method, both methods can be successfully applied for state estimator design. Moreover, these methods improve considerably the EKF performance when compared to a) the case of a constant-value and diagonal matrix Q in the presence of constant parametric uncertainty and to b) the methods of prior publications. Successive iterations of the Q tuning algorithm shall improve the state estimation accuracy. For the Williams-Otto semibatch reactor, only two iterations were necessary to improve the state estimation accuracy, significantly.

The main advantage of the algorithm presented in this work is that it is feasible for practical applications. Besides, of an online EKF tuning, the process model is updated online due to the integration of the state and the parameter estimation steps. Further, the algorithm eliminates an offline, exhaustive, and inexact tuning of EKF by trial and error.

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