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Unscented Kalman filters and Particle Filter methods for nonlinear state estimation

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Abstract

For nonlinear state space models to resolve the state estimation problem is difficult or these problems usually do not admit analytic solution. The Extended Kalman Filter (EKF) algorithm is the widely used method for solving nonlinear state estimation applications. This method applies the standard linear Kalman filter algorithm with linearization of the nonlinear system. This algorithm requires that the process and observation noises are Gaussian distributed. The Unscented Kalman Filter (UKF) is a derivative-free alternative method, and it is using one statistical linearization technique. The Particle Filter (PF) methods are recursive implementations of Monte-Carlo based statistical signal processing. The PF algorithm does not require either of the noises to be Gaussian and the posterior probabilities are represented by a set of randomly chosen weighted samples.

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1. Introduction

Many various problems in science and especially many various control algorithms require determination of the states for studied or controlled system. In more realistic cases only the outputs of the plant (rather than the state vector) can be measured. In this case the state estimation process often plays an important role in the process control

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implementation and in the monitoring applications. In case of the industrial processes there are many disturbing factors which influence the process control such as model and measurement uncertainties. In this paper we use the Gaussian probability distribution function to represent these uncertainties. The simple Kalman filter (KF) can be used only in case of linear dynamic systems and this algorithm propagates the mean and covariance of the probability distribution function of the model state in an optimal way. Almost all practical systems have some nonlinearity. If the studied system can be described with a nonlinear dynamic model than the most commonly used algorithm for the state estimation is the Extended Kalman Filter (EKF). In this case the state distribution is propagated analytically through a linear approximation of the system around the operating point at each time instant. This linear approximation may introduce errors in the estimated states, in other words with this method the results may not be appropriate for some systems. The Unscented Kalman Filter (UKF) is a derivative free method, and it resolves this problem by using a deterministic sampling approach. The Particle Filters (PF) method is a recursive implementation of the Monte Carlo based statistical signal processing. The aim of this work is to compare these state estimation methods for different nonlinear state space models.

Section 2 describes the principles of the nonlinear state estimation problem. The section 3 presents the general form of the of the EKF algorithm. Section 4 first introduces briefly the unscented transformation and after that the UKF algorithm. The section 5 presents the particle filter and the section 6 studies different examples to compare the performances of the EKF, UKF and PF algorithms. One of these examples is the nonlinear reactive magnetron sputtering process. Discussion of the results and the conclusions are presented in Section 6.

2. The nonlinear state estimation problem

To define the state estimation problem first we consider the general form of the discrete nonlinear process model, with *m* input signals, *p* output signals and the order of system is *n*. The discretization was made with sampling time T_s and we use the following notation for signal sequence $x_k = x(T_s \cdot k)$. In this reason the nonlinear discrete model is

$$\frac{\underline{x}_{k}}{\underline{y}_{k}} = F(\underline{x}_{k-1}, \underline{u}_{k-1}) + \underline{w}_{k-1}$$

$$y_{k} = \underline{G}(\underline{x}_{k}, \underline{u}_{k}) + \underline{y}_{k}$$
(1)

where $\underline{x}_k \in \mathcal{H}^n$ is the state vector, $\underline{u}_k \in \mathcal{H}^n$ is the system input vector and $\underline{y}_k \in \mathcal{H}^p$ is the noisy output vector of the system. The functions $\underline{F}: \mathcal{H}^n \to \mathcal{H}^n$ and $\underline{G}: \mathcal{H}^p \to \mathcal{H}^n$ are nonlinear and they need to be continuous. The w_k is one *n* dimensional process noise sequence and v_k is *p* dimensional observation (measurement) noise sequence. Both noises are Gaussian (normal distribution), independent random processes with zero means and known time invariant covariance matrices. If the E_{ij} is the expected value operator we can write:

$$w \sim N(0, \sigma_w) \qquad Q = \operatorname{cov}\{w\} = E\{w \cdot w^T\}$$

$$v \sim N(0, \sigma_v) \qquad R = \operatorname{cov}\{v\} = E\{v \cdot v^T\}$$

$$(2)$$

The objective of the estimation problem is to recursively estimate x_k from the output measurements y_k . In accordance with Bayes theory this mean, that recursively calculate the estimation of x_k at time k given the dates $y_1, ..., y_k$ up to time k. This is required calculation of the probability distribution function $pdf(x_k | y_{1k})$. We suppose that the initial pdf function of the state vector ($pdf(x_0 | y_0)$) is known and the $pdf(x_k | y_{1k})$ is obtained recursively in two sections: prediction step and update (correction) step.

3. The EKF algorithm for nonlinear state estimation

The Kalman Filter (KF) propagates the mean and covariance of the probability distribution function of the model state in an optimal way with minimization of the mean square error. The KF dynamics results from the consecutive cycles of prediction and filtering. The KF algorithm for state estimation can be applied just to the linear discrete time system model, when the model is nonlinear then we have to use the EKF algorithm. The EKF algorithm we

apply to the discrete nonlinear system model (1), where w_k and v_k are Gaussian distribution noises with known parameters (2). The extended algorithm is almost similar with KF algorithm, but in this case there was introduced one local linearization step of the model equations.

The steps of the EKF state estimation algorithm is presented below [1,5,12]:

0. Initialization step at k=0.

- Initial estimated state vector $\underline{\tilde{x}}_o = E\{\underline{x}_0\}$

- Initial covariance matrix: $\widetilde{P}_{0,x} = E\{(\underline{x}_0 - \underline{\widetilde{x}}_0) \cdot (\underline{x}_0 - \underline{x}_0)^T\}$

1. Local linearization step ($k \ge 1$): linearizing the nonlinear model functions F() and G() we can calculate the following matrices:

$$\Phi_{k} = \begin{bmatrix} \frac{\partial F_{1}}{\partial x_{1}} & \cdots & \frac{\partial F_{1}}{\partial x_{n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_{n}}{\partial x_{1}} & \cdots & \frac{\partial F_{n}}{\partial x_{n}} \end{bmatrix}_{\underline{x} = \underline{\tilde{x}}_{k-1}} C_{k} = \begin{bmatrix} \frac{\partial G_{1}}{\partial x_{1}} & \cdots & \frac{\partial G_{1}}{\partial x_{n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial G_{p}}{\partial x_{1}} & \cdots & \frac{\partial G_{p}}{\partial x_{n}} \end{bmatrix}_{\underline{x} = \underline{\tilde{x}}_{k-1}}$$
(3)

The linearization method utilizes just the first term in the Taylor expansion of the nonlinear functions 2. Prediction step: Calculation of the predicted state mean and covariance (time update)

$$\widetilde{\underline{x}}_{k}^{-} = F(\widetilde{\underline{x}}_{k-1}, \underline{u}_{k-1}) \qquad \widetilde{P}_{x,k}^{-} = \Phi_{k} \cdot \widetilde{P}_{x,k} \cdot \Phi_{k}^{T} + Q$$
(4)

3. Calculation of the filter gain vector:

$$K_k = \widetilde{P}_{x,k}^- \cdot C_k^T \cdot \left(C_k \cdot \widetilde{P}_{x,k}^- \cdot C_k^T + R\right)^{-1}$$
(5)

4. Correction step: The estimates are updated with latest observation (measurement update)

$$\widetilde{\underline{x}}_{k} = \widetilde{\underline{x}}_{k}^{-} + K_{k} \cdot (y_{k} - G(\widetilde{\underline{x}}_{k}^{-}, \underline{u}_{k})) \qquad \widetilde{P}_{x,k} = (I - K_{k} \cdot C_{k}) \cdot \widetilde{P}_{x,k}^{-}$$
(6)

The EKF gives an approximation of the optimal estimate. The non-linearities of the system's dynamics are approximated by a linearized version of the non-linear system model around the last estimated state [5]. This algorithm can be divergent if the consecutive linearizations are not a good approximation of the non-linear model.

4. The Unscented Transformation and UKF algorithm for nonlinear state estimation

Consider the non-linear system described by the equation (1). The state distribution is also represented by Gaussian random variables, but this method is using a minimal set of carefully chosen sample points. These points, called sigma points, completely capture the true mean and covariance of the states and are propagated through the nonlinearity. For calculating the statistics of a random variable which undergoes a nonlinear transformation we can use the unscented transformation (UT) [2, 4].

Consider a random variable x (dimension n), which is propagating through a nonlinear function y = f(x). The mean of x is $\overline{x} = E\{x\}$ and the covariance of x is $P_x = E\{(x - \overline{x}) \cdot (x - \overline{x})^T\}$. To calculate the statistics of y, we form a matrix \aleph of $2 \cdot n + 1$ sigma vectors according to the following:

$$\begin{split} \aleph_0 &= \overline{x} \\ \aleph_i &= \overline{x} + \gamma \cdot \left(\sqrt{P_x} \right)_i \quad i = 1, \dots, n \\ \aleph_i &= \overline{x} - \gamma \cdot \left(\sqrt{P_x} \right)_i \quad i = n+1, \dots, 2 \cdot n \end{split}$$
(7)

where $\gamma = \sqrt{n+\lambda}$ is a scaling parameter and $\lambda = \alpha^2 \cdot (n+k_f) - n$. The constant α determines the spread of the sigma points around the mean value \bar{x} and usually $\alpha \in [10^{-4}, 1]$. The constant k_f is a secondary scaling parameter and it is usually set to 0 for state estimation. $(\sqrt{P_x})_i$ is the i-th column of the matrix square root. These \aleph_i vectors are propagated through the nonlinear function $y_i = f(\aleph_i)$ $i = 0, ..., 2 \cdot n$. The mean and covariance for y are approximated using a weighted sample mean and covariance of the posterior sigma points:

$$\overline{y} \approx \sum_{i=0}^{2\cdot n} W_i^{(m)} \cdot y_i \qquad P_y \approx \sum_{i=0}^{2\cdot n} W_i^{(c)} \cdot (y_i - \overline{y}) \cdot (y_i - \overline{y})^T$$
(8)

The weights are given by

$$W_0^{(m)} = \lambda/(n+\lambda) \qquad W_0^{(c)} = \lambda/(n+\lambda) + (1-\alpha^2 + \beta) W_i^{(m)} = W_i^{(c)} = 1/(2 \cdot (n+\lambda)) \quad i = 1, \dots 2 \cdot n$$
(9)

where β is used to incorporate prior knowledge of the distribution of *x* (for Gaussian distribution the optimal value is 2). The standard UKF state estimation algorithm, with additive (zero mean) noise, is presented below [3,5]: 0. Initialization step at k=0:

- initial estimated state vector: $\underline{\widetilde{x}}_{o} = E\{\underline{x}_{0}\}$;

- initial covariance matrix: $\widetilde{P}_{x,0} = E\{(\underline{x}_0 - \underline{\widetilde{x}}_0) \cdot (\underline{x}_0 - \underline{x}_0)^T\}$. 1. Sigma points' calculation for k>=1

$$\aleph_{k-1} = \left[\widetilde{x}_{k-1} \quad \widetilde{x}_{k-1} + \gamma \cdot \sqrt{\widetilde{P}_{x,k-1}} \quad \widetilde{x}_{k-1} - \gamma \cdot \sqrt{\widetilde{P}_{x,k-1}} \right]$$
(10)

2. Propagation of the sigma points:

- transform the sigma points through the state-update function: $\aleph_k^* = F(\aleph_{k-1}, u_{k-1});$

- calculate the apriori state estimate and apriori covariance, where the weights $W_i^{(m)}$ and $W_i^{(c)}$ are defined in accordance with relations (9):

$$\widetilde{x}_{k}^{-} = \sum_{i=0}^{2n} W_{i}^{(m)} \cdot (\mathfrak{N}_{k}^{*})_{i} \qquad \widetilde{P}_{x,k}^{-} = \sum_{i=0}^{2n} W_{i}^{(c)} \cdot ((\mathfrak{N}_{k}^{*})_{i} - \widetilde{x}_{k}^{-}) \cdot ((\mathfrak{N}_{k}^{*})_{i} - \widetilde{x}_{k}^{-})^{T} + Q$$
(11)

.3. Update of the output vectors:

- transform the sigma points through the measurement-update function $Y_k^* = G(\aleph_{k-1}, u_k)$;

- calculate the mean and covariance of the measurement vector:

$$\widetilde{y}_{k}^{-} = \sum_{i=0}^{2 \cdot n} W_{i}^{(m)} \cdot (Y_{k}^{*})_{i} \qquad \widetilde{P}_{y,k}^{-} = \sum_{i=0}^{2 \cdot n} W_{i}^{(c)} \cdot ((Y_{k}^{*})_{i} - \widetilde{y}_{k}^{-}) \cdot ((Y_{k}^{*})_{i} - \widetilde{y}_{k}^{-})^{T} + R$$
(12)

4. Calculate the cross covariance matrix:

$$\widetilde{P}_{x,y,k} = \sum_{i=0}^{2n} W_i^{(c)} \cdot ((X_k^*)_i - \widetilde{x}_k^-) \cdot ((Y_k^*)_i - \widetilde{y}_k^-)^T$$
(13)

5. Calculation of the Kalman filter gain vector

$$K_k = \widetilde{P}_{x,y,k} \cdot (\widetilde{P}_{y,k}^-)^{-1} \tag{14}$$

6. Calculate the estimated state and the covariance in accordance with the standard Kalman filter algorithm:

$$\widetilde{\underline{x}}_{k} = \widetilde{\underline{x}}_{k}^{-} + K_{k} \cdot (y_{k} - \widetilde{y}_{k}^{-}) \qquad \widetilde{P}_{x,k} = \widetilde{P}_{x,k}^{-} - K_{k} \cdot \widetilde{P}_{y,k}^{-} \cdot K_{k}^{T}$$
(15)

The UKF principle is simple and easy to implement because it does not require the calculation of Jacobians at each time step [5]. The most computationally intensive operation in the UKF corresponds to calculating the new set of sigma points at each time update.

5. The Particle Filter algorithm

The Particle filter algorithms is a recursive implementation of the Monte Carlo based statistical signal processing method. The method approximates the Bayesian posterior probability density function (pdf) with a set of randomly chosen, weighted samples. Each sample of the state vector is referred to as a particle. A sufficiently large number of particles guarantee almost sure convergence to the true probability distribution function [6,7,8]. The discrete weighted approximation to the posterior pdf we can define

$$p(x_k \mid y_{1:k}) \approx \sum_{i=1}^{N_s} w_k^i \cdot \delta(x_k - x_k^i)$$
(16)

where δ () is the Dirac delta measure, the N_s is the number of samples, the $\{x_k^i | i = 1,...,N_s\}$ the set of random samples at time k, the $\{w_k^i | i = 1,...,N_s\}$ are normalized weights

$$\sum_{i=1}^{N_s} w_k^i = 1$$
(17)

The Sequential Importance Sampling (SIS) is the basic framework for particle filters: The main idea is to represent the required posterior density by a set of random samples with associated weights and to compute estimates based on these samples and weights [6]

$$w_{k}^{i} \propto w_{k-1}^{i} \cdot \frac{p(y_{k} \mid x_{k}^{i}) \cdot p(x_{k}^{i} \mid x_{k-1}^{i})}{q(x_{k}^{i} \mid x_{1:k-1}^{i}, y_{k})}$$
(18)

where $q(x_k|x_{1:k-l}, y_k)$ is the importance probability density function and ∞ is the proportionality symbol. A main problem with the SIS algorithm is the degeneracy phenomena, where after a few iterations; just one particle will have non negligible weight. This implies that a large computational effort is devoted to updating particles whose contribution to the approximation of $p(x_k|y_{1:k})$ is almost zero [6]. One measure of the degeneracy is the estimated value of the effective sample size:

$$N_{eff} = \left(\sum_{i=1}^{N_s} (w_k^i)^2\right)^{-1}$$
(19)

Serious degeneracy is indicated when the N_{eff} is small and $N_{eff} \leq N$. The degeneracy phenomena can be reduced with a good choice of the prior density function and if we use different resampling method. The importance resampling algorithm consists in choosing the prior density $p(x_k|x_{k-1})$ as importance density $q(x_k|x_{1:k-1},y_k)$, in accordance with that we can write:

$$w_k^l \propto w_{k-1}^l \cdot p(y_k \mid x_k^l) \tag{20}$$

The basic idea of resampling is to eliminate particles what have small weights and to concentrate on particles with large weights. In the literature are several method to solve this problem: multinomial resampling, residual sampling, systematic resampling, etc.

The particle filter algorithm for state estimation is presented below [7]:

- 1. *Initialization* (k=0): Set the initial state vector $\{x_0^i | i = 1,...,N_s\}$ and weights $w_0^i = 1/N_s$, $i = 1,...,N_s$ (assuming with that the all particles are equally probable at the start of the algorithm).
- 2. *Measurement update*: Update the weights $w_k^i = w_{k-1}^i \cdot p(y_k | x_k^i)$, whit normal probability density function (normpdf) and normalize the weight $w_k^i = w_k^i / \sum w_k^i$.
- 3. *Resampling*: apply the chosen resampling method (if the degeneracy phenomen is serious) to the set of particles $\{x_k^i | i=1,...,N_s\}$ and their weights $\{w_k^i | i=1,...,N_s\}$ to obtain a new set of particles and set of weights.
- 4. *Compute the estimate* :

$$\widetilde{\underline{x}}_{k} = \sum_{j=1}^{N_{s}} w_{k}^{j} \cdot x_{k}^{j}$$
(21)

5. Set k = k+1, and iterate the algorithm to step 2 at end of the simulation time interval.

6. Simulation studies

In this section we present some example and simulation results to compare the different characteristics of the three nonlinear state estimation method EKF, UKF and PF algorithms. The simulations of the estimation algorithms were made for three different types of systems. First we test this estimation algorithm for one theoretical nonlinear system, where we introduce different nonlinearities in observation model and at the end we test the presented algorithms to one complicate nonlinear system models (reactive sputtering system model). The numerical algorithms were implemented in Matlab environment. In all examples the simulations have been made in the following conditions:

- the process noise and measurement noise are applied to the system, both noises are Gaussian with zero mean and with known standard deviation ($w \sim N(0, \sigma_w)$, $v \sim N(0, \sigma_v)$);

- the initial values (the initial state vector and the initial covariance matrix), the process noise and measurement noise covariance matrices are chosen to be the same for all algorithms (EKF and UKF):

$$\widetilde{P}_{x,0} = \sigma_x^2 \cdot I_n \quad Q = \sigma_w^2 \cdot I_n \quad R = \sigma_v^2 \cdot I_p \tag{22}$$

- for PF algorithm the initial state vector is a Gaussian distribution vector with $\underline{\tilde{x}}_0 \sim N(\mu_x, \sigma_x)$;

- the measurements update sampling time of the Kalman filters coincides with the system sampling time (Ts);

- for the UKF algorithm the scaling parameters are set to the following values: $\alpha = 1$, $\beta = 2$, $k_f = 0$;

- for PF algorithm the number of particle will be notated by N_s and the resampling method is the systematic resampling method.

To compare the performances of the three approaches we can calculate the cumulative square error for every case (separately for each state). We can use the following relationship:

$$E_{i} = \frac{1}{N} \left(\sum_{j=1}^{N} (x_{i,j} - \widetilde{x}_{i,j})^{2} \right) \quad i = 1, ..., n$$
(23)

where n is the number of states and N is the number of samples.

6.1. Nonlinear theoretic system:

For comparison of the three approaches consider the following nonlinear systems:

$$\begin{aligned} x_{1,k} &= 0.5 \cdot x_{1,k-1} + x_{2,k-1} \cdot u_{k-1} + w_{1,k-1} \\ x_{2,k} &= -0.05 \cdot x_{1,k-1} \cdot x_{2,k-1} + u_{k-1} + w_{2,k-1} \end{aligned}$$
(24)

The estimation algorithms were tested first with one linear output function, in this case is.

$$y_k = 2 \cdot x_{1,k} - x_{2,k} + v_k \tag{25}$$

and after that with one nonlinear output function:

$$y_k = -x_{1,k} \cdot x_{2,k} + v_k \tag{26}$$

For both case the initial state and the tuning parameters are: $\sigma_x = \sqrt{10}$, $\sigma_v = \sqrt{4}$, $\sigma_w = \sqrt{0.1}$, $\mu_x=0$ and N_s=300, and the input is a variable step signal. The real measured output with noise and without noise and the estimated outputs using the EKF, UKF and PF algorithms, when the output is calculate with linear function (25) are shown in Fig.1 a. The cumulative square presented in Fig.1.b. The real states (non-measurable values with noises and without noises) and the estimated states using the EKF, UKF and PF algorithms when the output is calculate with nonlinear function (26) are shown in Fig.2, the cumulative square error Fig.3. We can observe the essential error value in case of EKF algorithm.



Fig.1. The measured outputs with noises and without noises and the estimated outputs using the EKF, UKF and PF algorithms (a), the cumulative square error (b) when the output function is linear



Fig.2 Estimated states x1 (a) and x2 (b) using EKF, UKF and PF algorithms for the when the output function is nonlinear



Fig.3. The cumulative square error for x_1 (b) and for x_2 (b) when the output function is nonlinear

6.2. Reactive sputtering process

In this section we try to use the presented estimation algorithms for one complex analytic nonlinear system model, what characterized the reactive sputtering process. A very sensitive aspect of the reactive sputtering process is the dynamic equilibrium of the reactive gas inside the chamber and of the metal atoms which form the compound with the reactive gas atoms on the surface of the substrate [9,10,11]. The dynamic model of the reactive magnetron sputtering process is defined by the system of equations [12]:

$$\frac{dp_N}{dt} = k_1 \cdot (q_{in} - q_p - (\alpha_{tM} \cdot F_N \cdot (1 - \theta_t) \cdot A_t + \alpha_{cM} \cdot F_N \cdot (1 - \theta_c) \cdot A_c)$$

$$\frac{d\theta_t}{dt} = \frac{1}{N_{Ti}} (2 \cdot \alpha_{tM} \cdot F_N \cdot (1 - \theta_t) - J \cdot \eta_N \cdot \theta_t)$$

$$\frac{d\theta_c}{dt} = \frac{1}{N_{Ti}} (J \cdot \eta_N \cdot \theta_t \cdot \left(\frac{A_t}{A_c}\right) \cdot (1 - \theta_c) + 2 \cdot \alpha_{cM} \cdot F_N \cdot (1 - \theta_c) - J \cdot \eta_M \cdot (1 - \theta_t) \cdot \left(\frac{A_t}{A_c}\right) \cdot \theta_c)$$
(27)

In this mathematical model the following notation and numerical parameters values has been used: p_N - the partial pressure of reactive gas (nitrogen) in the sputtering chamber; θ_r - the fractional surface of the target covered by compound molecules;

 θ_c - the fraction of the condensation area covered by compound molecules;

 F_N - the flux of reactive gas molecules (N₂) on the target or on the substrate ($F_N = k_1 p_N$);

 q_{in} - the input reactive gas flow;

 q_p - the gas flow evacuated by the vacuum pump;

 $A_t A_c$ - the target area (0.84 1e-2 m²) and the substrate (condensation) area (0.22 m²);

 $m_N m_{T_1}$ mass of the reactive gas molecule (28 a.u) and of the metal (47.9 a.u.) (1.a.u.=1.66 le-27 kg);

 η_M , η_M sputtering yield of the elemental (Ti) metallic (1.5) and of the compound (titanium nitride) material (0.3);

 $\alpha_{\ell M}, \alpha_{\ell M^-}$ sticking coefficients for the nitrogen molecule (to the titanium target or to the covered part);

 N_{Tr} the superficial density of the titanium atoms on the surface of the metallic target (140 le-12 m⁻²);

J- the particle density of argon ions on the surface of the target, which can be calculated using the relationship $J=I_d/(A_t e)$, where *e* is the charge of electron (1.6 le-19 C) and I_d is the intensity of the discharge current;

 k_{1} - proportional coefficient, calculated in function of temperature and chamber volume.

R – ideal gas constant (8314 J/molK);

 N_A – Avogadro's number (6.022 1e23 mol⁻¹);

T – temperature (300K);

V – volume of the sputtering chamber (75 1e-3 m³).

This mathematical model in state space representation has three state variables $(x_1=p_N, x_2=\theta_t and x_3=\theta_c)$ two input signals $(u_1=q_{in} \text{ and } u_2=I_d)$ and for the output signal we can choose between the fractional surface of the target θ_t , the fractional surface of the condensation area θ_c covered by compound molecules, but we can also chose the pulverization rate (R_p) or the speed of deposition (a_p) what can be calculate with following nonlinear relationships.

$$R_p = J \cdot (\eta_N \cdot \theta_t + \eta_M \cdot (1 - \theta_t)) \qquad a_D = \frac{m_{T_i} \cdot R_p \cdot A_t}{\rho_{T_i} \cdot A_c} \cdot \xi$$
(28)

where ρ_{Ti} is the metal density (4.51 1e3 kg/m³) and ξ is one accommodation coefficient (0.8).

The reactive sputtering process has been simulated employing a Runge-Kutta step control algorithm. The sampling time was typically set to 0.001 sec, and the initial states vector: [4e-3 0.09 0.37]. For this case the numerical simulation has following parameters:

 $\sigma_x = [1e-4 \quad 1e-2 \quad 1e-2]; \sigma_w = [1e-5 \quad 1e-2 \quad 1e-3]; \sigma_v = 1e-2; \quad \mu_x = x_0, \quad N_s = 100$ The first input signal (q_{in}) is one step variable signal and the second input (I_d) is constant. First the output is set $y = \theta_c$ and at the second case the output is $y = a_D$. Simulation results for the first case are presented in Fig.4.



Fig.4. The measured and estimated outputs with EKF, UKF and PKF algorithms (a) and the cumulative errors (b) when $y=x_3$

When the output is the a_D that is mean that the output function is also nonlinear, the EKF results is worst but results in case of PF and UKF are more better (Fig.5).



Fig.5. The measured and estimated outputs with EKF, UKF and PKF algorithms (a) and the cumulative errors (b) when $y=a_D$

7. Conclusion

This paper shows that the UKF and the PF algorithms for state estimation is an interesting alternative to the EKF because they have some improved performances. The PF and UKF methods are simpler to implement compared to EKF. The computational load of UKF is comparable to the EKF approach, where the Jacobians are computed numerically in each step of the algorithm. The performance of the PF depends of the number of particles. If this number is great then the calculation time is also significant in correlation with the others methods.

References

- Riberio MI. Kalman and Extended Kalman Filters, Concept, Derivation and Properties, Institute for Systems and Robotics, Instituto Superior Tecnico Lisboa ,2004. Available: http://users.isr.ist.utl.pt/~mir/pub/kalman.pdf.
- [2] Terejanu GA. Unscented Kalman Filter Tutorial, Department of Computer Science and Engineering University at Buffalo, Buffalo, NY. Available: http://users.ices.utexas.edu/~terejanu /files/tutorialUKF.pdf.
- [3] Van der Merwe R, Wan EA. The square-root unscented Kalman filter for state and parameter estimation, Oregon Graduate Institute of Science and Technology, Oregon, 2000. Available: http://www.researchgate.net/publicati on/2895916_The_Square-Root_Unscented_Kal man_Filter_for_State_and_Parameter-Estimition.
- [4] Wan EA, van der Merwe R. The Unscented Kalman filter. Available: http://stomach.v2.nl/Docs/TechPubs/Tracking_and_AR /wan01unscented.pdf.
- [5] Kandepu R, Foss B, Imsland L. Applying the unscented Kalman filter for nonlinear state estimation, Science Direct, Journal of Process control, 2008 [Online]. Available: http://www.itk.ntnu.no/ansatte/Foss_Bjarne/pubs/journals/journal-47.pdf.
- [6] Sanjeev Arulampalam M, Maskell S, Gordon N, Clapp T. A Tutorial on Particle filters for Oline Nonlinear/Non-Gaussian Bayesian Tracking, IEEE Transactions on signal Processing, 2002; 50(2): 174-188.
- [7] Alfonso Manya. Particle Filter and Extended Kalman Filter for Nonlinear Estimation: A comparative Study (2008), Available: http://users.isr.ist.utl.pt/~pjcro/cadeiras/dsfps0708/SEMS/PF EKF TermPaper.pdf.
- [8] Doucet A, Johansen A. A tutorial on Particle Filtering and Smoothing, 2008. Available: http://www.cs.ubc.ca/~arnaud/ doucet johansen tutorialPF.pdf.
- Berg S, Blom HO, Larsson T, Nender C. Modeling of reactive sputtering of compound materials, J.Vac. Sci. Technol., 1987; A5 (2): 202-207.
- [10] Berg S, Nyberg T. Fundamental understanding and modeling of reactive sputtering processes, Science direct, Thin Solid films, 2005; 476 (2): 215-230.
- [11] György K, Kelemen A, Papp S. Modeling and stability analysis of the nonlinear reactive sputtering process, Scientific Bulletin of the "Petru Maior" University of Tg. Mureş, 2011; 8 (2): 33-37.
- [12] Papp S, György K, Kelemen A, Jakab-Farkas L. Applying the Extended and Unscented Kalman Filters for Nonlinear State Estimation, Inter-Eng 2012 Conference Proceedings, Tg Mures, 2012: 233-239.