Simulation Study of the Particle Filter and the EKF for State Estimation of a Large-scale DAE-system with Multi-rate Sampling

Daniel Haßkerl, Momin Arshad, Reza Hashemi, Sankaranarayanan Subramanian, Sebastian Engell

Abstract: In the present contribution we study the application of the Particle Filter (PF) and of the Extended Kalman Filter (EKF) incorporating measurements at different sampling rates for the state estimation of a large-scale model. We investigate a model of an intensified chemical process (a reactive distillation (RD) process) that is represented by a nonlinear DAE-system and has more than 100 states. The EKF and PF schemes are studied for two different cases. The performance of each of the estimation method is compared first for the case where the estimator uses a model which is identical to the process. Secondly, the model used by the estimator is considered to be parametrically different from the model used to simulate the process. The effect of model-plant mismatch on the mean squared estimation error is studied for both state estimation methods. The goal is to give arguments for the selection of either of the methods to be used at the real process unit fulfilling the requirements of accurate estimation and real-time capability.

Keywords: Particle Filter, Extended Kalman Filter, state estimation, multi-rate sampling, nonlinear DAE-systems, reactive distillation.

1. INTRODUCTION

In chemical engineering, process intensification and process integration are general trends. In process integration, different operations, usually a reaction step and a separation step, are combined in a single apparatus. The approach is known to reduce the complexity of the process and the energy demand due to making use of fewer pieces of equipment and exploiting synergies. Process integration leads to complexity when referring to mathematical modelling of these process units and thus poses a challenge for the application of model-based control techniques to these units. Reactive distillation is an example of such an intensified process for which accurate mathematical models that capture the steady-state and dynamic behavior of the underlying intensified process exist. For reactive distillation processes, these models contain a large number of state variables. Among the possibly hundreds of states, usually only a small number of variables can be measured. However, for model-based control, information on the full state vector of the underlying mathematical model has to be provided. In the case of an observable process, this demand can be met by state estimation techniques, which use the measured output and the dynamic model to compute the state of the underlying process. In chemical processes, it must be considered that the measurements often are available at different sampling rates. These differences usually arise from the offline-analysis of samples in the laboratory or the measurement of concentrations which require significant post-processing. Therefore, state estimator formulations that are capable of handling multi-rate sampling have been presented in the literature. These formulations can deal with mathematical models that are based on ordinary differential equations (ODE) and differential algebraic equations (DAE) (see among others, Simon (2006), Krämer and Gesthusien, (2005)). Krämer and Gesthusien et al., (2006) and Purohit (2014) have reported good results for the application of multi-rate state estimation techniques such as the moving horizon estimator (MHE) and the Extended Kalman Filter (EKF). For the EKF, some assumptions on the statistical properties of the state and measurement noise are made (independent Gaussian white noise signals) and the EKF uses simplifications such as linearization of the process model and of the measurement equation for the propagation and the update of the error covariance (Simon (2006)). The computational advantage resulting from the aforementioned simplifications has led to real applications in the chemical industry, e.g. see (Finkler et al., (2012), Auger et al., (2013)). These assumptions and simplifications are not made in probability-based state estimation techniques as e.g. Particle Filters (PF) and thus good results for state estimation problems of ODE-systems are also obtained (Hashemi and Engell, (2014))). Here we investigate the DAE-EKF and the DAE-PF using the multi-rate formulation for a reactive distillation case study from (Keller et al., (2012) and Keller (2012)). The process under consideration is the transesterification of dimethyl carbonate (DMC) with ethanol (EtOH) in a pilot-scale reactive distillation column. In the
experimental work, samples for the off-line analysis of the liquid composition profile were taken at time instances that differed from other measurements such as pressure, temperatures and flows which were available online. Besides providing experimental data, the authors presented different DAE-models of the process. We here use one of the simpler models. In a first step, we study the estimation methods for the state estimation under the assumption, that no model-plant mismatch is present. Secondly, we consider that the process model is subject to parametric model-plant mismatch that is not considered in the model of the estimator. The performance of each of the estimators is studied and the effect on the mean squared estimation error is discussed.

The paper is structured as follows: In section 2, the mathematical model of the process is introduced. Section 3 deals with the two state estimation techniques. The estimation results for multi-rate state estimation with and without model-plant mismatch are presented in section 4. Finally conclusions and an outlook on future work follows in section 5.

2. MATHEMATICAL PROCESS MODEL

In Fig. 1, a schematic representation of the reactive distillation column for the transesterification process is shown (adapted from Keller et al., (2012)). The reactive distillation column can be subdivided into a stripping section (black, below the feed) and a rectifying section (grey, above the feed). Inside the reactive distillation column, a two-step transesterification reaction takes place in the liquid phase of the stripping section.

**Figure 1:** Schematic representation of the reactive distillation column for the transesterification process

Transesterification of Dimethyl Carbonate with Ethanol:

Transesterification of Ethyl-Methyl Carbonate with Ethanol:

The reaction scheme consists of the formation of ethyl methyl carbonate (EMC) in a first step and the formation of diethyl carbonate (DEC) in a second step. Methanol is a byproduct of the reaction. Keller et al., (2012) have investigated the process experimentally and developed detailed mathematical models of different complexity using the MESH (Material, Equilibrium, Summation, Enthalpy or Heat balance) equations. From the set of the models presented in Keller et al., (2012), the EQ-Kin (equilibrium-stage model using reaction kinetics) model is selected as the process model for state estimation here. The EQ-Kin model incorporates equations for each section of the process, the condenser, the reboiler, the liquid distributors and the packing sections. The packing is axially discretized and for each discrete element, an equilibrium stage model is used. In this work, it is assumed that each packing section can be represented by a single equilibrium stage model. The mathematical formulation of the model of the reactive distillation column using the MESH equations then results in a set of 65 differential and 170 algebraic equations. Correlations for thermophysical parameters, equilibrium calculations using UNIQUAC, hold-up and pressure drop correlations are used (see Keller et al., (2012) and Keller (2012) for details on the MESH model).

For state estimation, the mathematical model can be represented as a general dynamic discrete-time DAE system

\[
x_{k+1} = f(x_k, z_k, w_k)
\]

\[
o = g(x_k, z_k)
\]

\[
y_k = h(x_k, z_k, v_k)
\]

where \( w_k \in \mathbb{R}^{n_w} \) and \( v_k \in \mathbb{R}^{n_v} \) are independent white noise sequences with known probability density functions (pdf), and \( x_k \in \mathbb{R}^{n_x} \) and \( z_k \in \mathbb{R}^{n_z} \) are the differential and algebraic states and \( y_k \in \mathbb{R}^{n_y} \) represents the measurements at the time instance \( k \). The inputs \( u_k \in \mathbb{R}^{n_u} \) are initialized with the inputs corresponding to experiment E13 (cf. Keller et al., (2012)) and are kept constant in the simulations. The state vector is aggregated as

\[
s_k = [x_k, z_k]^T,
\]

where \( s_k \in \mathbb{R}^{n_w+n_z} \) consists of both differential and algebraic states. The process noise of the differential states describing the temperatures is assumed to have a standard deviation of \( 1.0 \times 10^{-4} \) with zero mean, while the process noise of the rest of the differential states is assumed to have a standard deviation of \( 1.0 \times 10^{-5} \) with zero mean.

<table>
<thead>
<tr>
<th>Name</th>
<th>Measured state</th>
<th>Packing height</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid Distributor 1</td>
<td>Vapor temperature</td>
<td>5.4 m</td>
</tr>
<tr>
<td>Liquid Distributor 2 (LD2)</td>
<td>Vapor temperature</td>
<td>4.2 m</td>
</tr>
<tr>
<td>Liquid Distributor 3</td>
<td>Vapor temperature</td>
<td>3.0 m</td>
</tr>
<tr>
<td>Liquid Distributor 4</td>
<td>Vapor temperature</td>
<td>1.0 m</td>
</tr>
<tr>
<td>Liquid Distributor 5</td>
<td>Vapor temperature</td>
<td>0.5 m</td>
</tr>
<tr>
<td>Liquid Distributor 6 (LD6)</td>
<td>Vapor temperature</td>
<td>0.0 m</td>
</tr>
<tr>
<td>Reboiler</td>
<td>Vapor and liquid temperature, liquid composition, volume</td>
<td>Below the packing</td>
</tr>
</tbody>
</table>

The measurement noise of the temperatures is assumed to have a standard deviation of \( 4.0 \times 10^{-5} \) with zero mean, while the state noise of the rest of the differential states is assumed to have a standard deviation of \( 1.0 \times 10^{-5} \) with zero mean. The available measurements and their position are collected in...
Table 1. For the study of the parametric uncertainty, it is assumed that the reaction equilibrium constant of the first reaction chain is increased by 15% compared to the nominal case. This increase of the parameter affects the reaction equilibrium in the liquid phase of the stripping section of the reactive distillation column. The effect of this type of plant-model mismatch is not serious and slightly modifies the transient behavior of the underlying process.

In the second case, the plant-model mismatch is represented by a 10% decrease of the pressure at the top of the column. This noticeably affects the vapor liquid equilibrium (VLE) throughout the column.

The mathematical models are formulated and implemented in Matlab 2011b. For numerical solution, the routine ODE15s using default settings was chosen. The Jacobians are approximated using central differences.

3. STATE ESTIMATION

3.1 Particle Filter Algorithm for Single-Rate Sampling

Here we describe the algorithm of Particle Filter shortly. Detailed descriptions can be found in (Li et al., 2015), Simon (2006), Doucet et al., (1998), Karlsson (2012), Arulampalam et al., (2002) and Orhan (2012). The algorithm starts by generating \( N \) initial particles from the known pdf of the initial conditions. We denote these particles by \( s^*_{0,i} \). Each particle is a candidate set of states of the system and generally more particles result in better estimation accuracy and prevents sample degeneracy and sample impoverishment (Arulampalam et al., 2002). The particles are propagated and the measured variables are computed for them and based on these computed variables, a weight is assigned to each particle. Of the next sampling instance are repeated. The particles of the next sampling instance are

Considering that \( n_x \) measurements are available and the measurements are subject to Gaussian noise, the weight of each particle is computed as

\[
q_i = p(\mathbf{y}_k | \mathbf{s}_{k,i}^*) \sim \frac{1}{\sqrt{2\pi R}} \exp \left( -\frac{1}{2} \mathbf{z}_k - h(\mathbf{x}_k) \mathbf{R}^{-1} \mathbf{z}_k - h(\mathbf{x}_k) \mathbf{R}^{-1} \mathbf{z}_k \right),
\]

where \( R \) is the covariance matrix of the measurement noise.

Once the weights of all the particles are computed, the algorithm chooses a set of a posteriori particles by replacing the particles with negligible weights with particles that have larger weights and the mean of this set is the current state estimate. This procedure is called resampling and the selected set contains exactly \( N \) particles where a subset of the particles is repeated. The particles of the next sampling instance are built from the particles of this set. Usually the number of distinct particles in the resampled set is small and therefore the set will lose its diversity and cannot represent the pdf of the states. This problem is called sample impoverishment and a common approach to overcome this problem is roughening in which random noise is added to the resampled particles to increase the diversity of the particles for the next iteration.

3.2 Extended Kalman Filter for Single-Rate Sampling

Unlike the particle filter, the EKF relies on linearization with first order accuracy (bold letters correspond to vector and matrix notation). By setting the matrices \( A_k, B_k, C_k \) and \( D_k \) as follows

\[
A_k = \frac{\partial f}{\partial \mathbf{x}^k(\mathbf{x}_k, \mathbf{z}_k)}, \quad B_k = \frac{\partial f}{\partial \mathbf{u}^k(\mathbf{x}_k, \mathbf{z}_k)},
\]

\[
C_k = \frac{\partial g}{\partial \mathbf{x}^k(\mathbf{x}_k, \mathbf{z}_k)}, \quad D_k = \frac{\partial g}{\partial \mathbf{u}^k(\mathbf{x}_k, \mathbf{z}_k)},
\]

a linearized approximation of the discrete-time DAE system can be obtained (Mandela et al., 2010)

\[
\bar{\mathbf{s}}_{k+1} = \mathbf{A}_{k}^{aug} \mathbf{s}_k,
\]

where

\[
\mathbf{A}_{k}^{aug} = \begin{bmatrix} A_k & B_k \\ -D_k^T C_k A_k & -D_k^T C_k B_k \end{bmatrix}
\]

The matrix \( \mathbf{A}_{k}^{aug} \) is used in the computation of the time update of the covariance matrix. For the algorithm of the single-rate DAE-EKF for the prediction and update step, please refer to the upcoming section.

3.3 Multi-rate Sampling

Consider that the available set of measurements at the faster sampling-rate is \( \mathbf{y}_k \) while the rest of the measurements are available at a slower sampling rate \( \mathbf{y}_k^s \). It is assumed that the slower sampling rate is a multiple of the faster sampling rate \( i \). Therefore at the major sampling instant, all measurements are available and the algorithm of the Particle Filter reads as for the single-rate sampling scenario. The measurement equation at the major sampling instant is thus given by

\[
\mathbf{y}_k = \mathbf{h}(\mathbf{x}_k, \mathbf{z}_k, \mathbf{v}_k)
\]

However, at the minor sampling instant, only the measurements at faster sampling rate are available. The modified measurement equation is given by

\[
\mathbf{y}_k^s = \mathbf{h}^s(\mathbf{x}_k, \mathbf{z}_k, \mathbf{v}_k)
\]

In the Particle Filter, the computation of the relative likelihood \( q_i \) of the particles changes as follows (see (Häkkinen et al., 2016))

\[
q_i = p(\mathbf{y}_k^s | s_{k,i}^*),
\]

\[
\sim \frac{1}{n_y} \exp \left( -\frac{1}{2} \left[ h^s(\mathbf{s}_{k,i}^*) \mathbf{R}^{-1} \left[ h^s(\mathbf{s}_{k,i}^*) \right] \right] \right)
\]

The formulation of the extension of the EKF for the multirate case has been done based on (Simon 2006). The linearized measurement model is computed according to

\[
\mathbf{H}_k^s = \frac{\partial \mathbf{y}_k}{\partial \mathbf{s}} \bar{\mathbf{s}}_k
\]
The computation of the Kalman gain of the state estimates and of the updated error covariance matrix for the major and the minor sampling instances are shown in Algorithm 1.

Note, that for simulation and estimation, the inputs are kept constant, thus they are not explicitly shown in the algorithm.

4. RESULTS

The estimation results using the multi-rate formulations of the EKF and of the PF are presented in this section. It is assumed that the vapor phase temperatures on each liquid distributor are available every second, whereas the composition on the top and the bottom of the RD column are available every 30 seconds (i.e., 30 in all cases). The tuning parameters used for the extended Kalman filter are

\[
Q_1 = 1 \times 10^{-4}, \quad Q_2 = 1 \times 10^{-7} \\
R_1 = 4 \times 10^{-2}, \quad R_2 = 1 \times 10^{-5} \\
P_{01} = 1 \times 10^{-4}, \quad P_{02} = 1 \times 10^{-7}.
\] (12)

The tuning parameters of the PF (50 particles) are

\[
R_{N1} = 5 \times 10^{-3}, \quad R_{N2} = 5 \times 10^{-4} \\
R_1 = 4 \times 10^{-2}, \quad R_2 = 1 \times 10^{-5} \\
P_{01} = 1 \times 10^{-4}, \quad P_{02} = 1 \times 10^{-7}.
\] (13)

Note that in the case of the EKF, each diagonal element of \( Q \) related to the liquid and vapor temperature is denoted by \( Q_1 \) whereas each diagonal element of \( Q \) related to the remaining states is denoted by \( Q_2 \). In the same way, each diagonal element of \( R \) corresponding to temperature measurement is denoted by \( R_1 \) whereas each diagonal element of \( R \) corresponding to the remaining measurements (concentrations and reboiler holdup) is denoted by \( R_2 \). Similarly, the diagonal elements of the matrix \( P_0 \) corresponding to all vapor and liquid temperature states are chosen to be equal and their diagonal elements are denoted by \( P_{01} \), whereas the diagonal elements of the matrix \( P_0 \) for all remaining states are chosen to be equal and their diagonal elements are denoted by \( P_{02} \).

Furthermore, in the case of the Particle Filter, the roughening noise added to all the particles related to the vapor and liquid temperature states are chosen the same and the standard deviation of roughening noise added to these particles is denoted by \( R_{N1} \), whereas the roughening noise added to all the particles related to the remaining states are chosen the same and the standard deviation of roughening noise added to these particles is denoted by \( R_{N2} \).

Throughout this section, the solid lines correspond to the simulated states, the dashed lines correspond to the state estimates and the dotted lines represent the measured states.

4.1 State estimation for the nominal case

The state estimation results using the multi-rate DAE-EKF and the multi-rate DAE-PF without plant-model mismatch are shown in Fig. 2 and 3.

![Figure 2: State estimation results of the multi-rate DAE-EKF applied to the case study (no plant-model mismatch considered)](image)

![Figure 3: State estimation results of the multi-rate DAE-PF applied to the case study (no plant-model mismatch considered)](image)
compared to the EKF. This discrepancy increases after the initial convergence, so that the estimation error is up to 26-fold worse. Even though the initial pdf of the particles is reasonably good, using only 50 particles is not enough to approximate the pdf of the plant with more than 200 states. This problem could be solved by using more particles, but this would further increase the computation time.

Table 2: Comparison of the mean squared estimation error using extended Kalman filter and particle filter on the case study (no plant-model mismatch considered).

<table>
<thead>
<tr>
<th>State Estimator</th>
<th>EMC (till 200s) (×10^{-6})</th>
<th>EMC (after 200s) (×10^{-6})</th>
</tr>
</thead>
<tbody>
<tr>
<td>EKF</td>
<td>8.16</td>
<td>1.64</td>
</tr>
<tr>
<td>PF (N=50)</td>
<td>32.85</td>
<td>16.08</td>
</tr>
</tbody>
</table>

4.2 State estimation under plant-model mismatch (increase of the reaction equilibrium constant)

The state estimation results using the EKF on the case study with the plant-model mismatch (increase of reaction equilibrium constant by 15%) are presented in Fig. 4.

Due to the plant-model-mismatch, most of the estimation results become less accurate but still acceptable. Specifically in the case of the EMC liquid phase composition at liquid distributor five and six, the mismatch between the simulated plant data and the estimation results is noticeable. No measurement is assumed to be present and thus the state estimates rely on the temperatures of the vapor phase only. The state estimation results using the PF for the same case are presented in Fig. 5. The effect of the parametric plant-model mismatch on the state estimation using the PF is noticeable.

Table 3 summarizes the mean squared estimation error of selected EMC and DEC liquid phase compositions using the EKF and the PF and Fig. 6 depicts the mean squared estimation error relative to the EKF.

4.3 State estimation under plant-model mismatch (decrease of the pressure)

Fig. 7 depicts the state estimation results of the Extended Kalman Filter that is applied to the case study with plant-model mismatch (decrease of the pressure at the top of the column). It can be seen that the state estimation results are quite poor. However, this is an expected behavior as the plant-model mismatch is serious and the EKF employs a model with a wrong dynamic behavior paired with usage of the linearization of the model equations. For the same case,
the estimation results using the multi-rate PF (N=50) completely failed to converge and merely follows the horizontal line of the initial state estimates (results not shown). 50 particles are not diverse enough to approximate the pdf of the states. Fig. 8 depicts the case when the number of particles is chosen to be 500 (RN1 = 5×10^-2, RN2 = 5×10^-3 and P01 = 1×10^-2, P02 = 1×10^-3), which converges.

Figure 7: State estimation results of the multi-rate DAE-EKF applied to the case study with plant-model mismatch (decrease of pressure at the top of the column)

![Graph showing liquid and vapor phase compositions and temperature over time with a liquid distributor](image1)

Figure 8: State estimation results of the multi-rate DAE-PF applied to the case study with plant-model mismatch (decrease of pressure at the top of the column), N=500

The relative mean squared error for this case is depicted in Fig. 9. The estimation error of the DAE-EKF and of the DAE-PF using 500 particles are ten-fold higher in case of serious plant-model mismatch. The EKF outperforms the PF in almost all cases (cf. Fig. 9, only one exception) and is at the same time computationally cheap (each estimation step required approximately 850 seconds for the Particle Filter with 500 particles, whereas the EKF required approximately five seconds).

5. CONCLUSIONS

The state estimation using multi-rate DAE-PF is computationally demanding as compared to the DAE-EKF, which employs a linearized model. In all cases considered in this work, the DAE-EKF shows a similar performance as compared to the DAE-PF with much smaller computational cost. For this process, DAE-EKF is favorable because it is real-time implementable and the required accuracy of the estimation is achieved.

![Graph showing mean squared estimation error over time](image2)

Figure 9: Mean squared estimation error of the Particle Filter relative to the EKF (plant-model mismatch: 10% decrease of the pressure)

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