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Simulation Study of the Particle Filter and the EKF for State Estimation of a Large-scale DAE-system with Multi-rate Sampling[1]

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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 complexification 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 Gesthuisen, (2005)). Krämer and Gesthuisen 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

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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

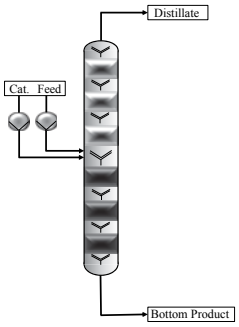


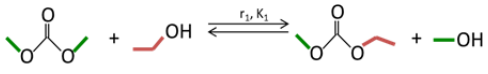
Figure 1: Schematic representation of the reactive distillation column for the transesterification process

In Fig. 1, a schematic representation of the RD-process for the transesterification of dimethyl carbonate with ethanol considered in this work is shown (adapted from Keller et al., (2012)).

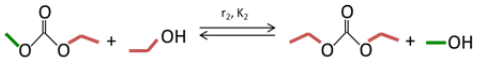
The reactive distillation column can be subdivided into a stripping section (black, below the feed) and a rectifying section (grey, above the feed).

Inside the reactive distillation column, a homogeneously catalyzed two-step transesterification reaction takes place in the liquid phase of the stripping section.

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

$$\begin{aligned} \boldsymbol{x}_{k+1} &= \boldsymbol{f}(\boldsymbol{x}_k, \boldsymbol{z}_k, \boldsymbol{w}_k) \\ \boldsymbol{0} &= \boldsymbol{g}(\boldsymbol{x}_k, \boldsymbol{z}_k) \\ \boldsymbol{y}_k &= \boldsymbol{h}(\boldsymbol{x}_k, \boldsymbol{z}_k, \boldsymbol{v}_k) \end{aligned} \tag{1}$$

where $\boldsymbol{w}_k \in \mathbb{R}^{n_x}$ and $\boldsymbol{v}_k \in \mathbb{R}^{n_y}$ are independent white noise sequences with known probability density functions (pdf), and $\boldsymbol{x}_k \in \mathbb{R}^{n_x}$ and $\boldsymbol{z}_k \in \mathbb{R}^{n_z}$ are the differential and algebraic states and $\boldsymbol{y}_k \in \mathbb{R}^{n_y}$ represents the measurements at the time instance k. The inputs $\boldsymbol{u}_k \in \mathbb{R}^{n_u}$ 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

$$\boldsymbol{s}_k = [\boldsymbol{x}_k, \boldsymbol{z}_k]^T, \tag{2}$$

where $\boldsymbol{s}_k \in \mathbb{R}^{n_x+n_z}$ 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 1.0×10^{-4} with zero mean, while the process noise of the rest of the differential states is assumed to have a standard deviation of 1.0×10^{-7} with zero mean.

Table 1: Available RD-column measurements

Name	Measured state	Packing height
Liquid Distributor 1	Vapor temperature Liquid Composition	5.4 m
Liquid Distributor 2 (LD2)	Vapor temperature	4.2 m
Liquid Distributor 3	Vapor temperature	3.0 m
Liquid Distributor 4	Vapor temperature	1.0 m
Liquid Distributor 5	Vapor temperature	0.5 m
Liquid Distributor 6 (LD6)	Vapor temperature	0.0 m
Reboiler	Vapor and liquid temperature, liquid composition, volume	Below the packing

The measurement noise of the temperatures is assumed to have a standard deviation of 4.0×10^{-2} with zero mean, while the state noise of the rest of the differential states is assumed to have a standard deviation of 1.0×10^{-5} with zero mean. The available measurements and their position are collected in