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Effect of Sampling Rate on the Divergence of the Extended Kalman Filter for a Continuous Polymerization Reactor in Comparison with Particle Filtering ⋆

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Abstract: The Extended Kalman Filter (EKF) is the most widely used state estimation technique for non-linear systems in the field of process engineering. In this contribution, we investigate the performance of the EKF for continuous polymerization of acrylic acid in a tubular reactor with multiple side feeds of monomer. The EKF usually yields satisfactory estimations if the nonlinearities of the underlying system are not too severe. We observed that the EKF for this process diverges regardless of its tuning unless it is iterated at very fast sampling rates. In order to verify this, we have tested the EKF for different tunings and different sampling rates in 100 independent Monte Carlo simulations for each setup. In contrast Particle Filters use the nonlinear model of the process directly and do not suffer from the problems caused by linearization. On the other hand the computation times are significantly higher.

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1. INTRODUCTION

State estimation is an important part of every model-based control system. In such a control scheme, the controller simulates the process model to compute the optimal inputs (according to some cost function, tracking or economics-based) and therefore the process states are needed to initialize the model. Usually not all states of a system are measurable. The high price of reliable sensors is one of the reasons to implement state estimators. Also sometimes the process does not have a proper configuration to install the necessary sensors or for some quantities sensors cannot provide the measurements at the requested frequency or not accurately enough. Even in the case of the availability of measurements, they are always contaminated with noise. These reasons make it indispensable to implement state estimation techniques in model-based control systems.

All state estimation techniques utilize a model of the underlying process and use the measured control inputs and the available state measurements to reproduce the states. For linear systems, the Luenberger observer and the Kalman Filter are the most widely used state estimation techniques. In the area of the non-linear systems, the Extended Kalman Filter (EKF), Unscented Kalman Filter (UKF), high gain observers, Moving Horizon Estimators (MHE), Particle Filtering (PF) and many others have been proposed. Due to its relatively simple structure and low computation effort, the Extended Kalman Filter is the most popular estimation technique for non-linear systems. This state estimation technique employs the non-linear model of the process in the prediction step but uses a linearized model in the computation of the correction gain and of the error covariance matrix. It is well known that the performance of the EKF is determined to a large extent by the tuning of its free parameters Q, R and $P(0)$, where Q and R are the covariance matrices of the process noise and the measurement noise and $P(0)$ is the error covariance of the initial states. For complex systems which comprise hundreds of states and where usually the number of the available measurements compared to the number of the states is small, tuning of these parameters can be a difficult task. The Extended Kalman Filter usually exhibits a satisfactory performance if the non-linearities of the system are not too severe, otherwise the estimator may diverge.

In this contribution we demonstrate for a practically relevant example that the Extended Kalman Filter diverges unless the sampling times are very short and compare it with a Particle Filter. Particle Filters implement the non-linear model of the process directly and do not suffer problems caused by the linearization. We compare these two estimation techniques in terms of the effect of the sampling rate on the convergence and with respect to the computation times.

The rest of this paper is organized as follows: In section 2 the process model, its properties and the numerical method to solve it are discussed. Section 3 describes the Extended Kalman Filter and its performance for our test case. The Particle Filtering and the estimation results using this technique for the tubular reactor example are presented in section 4. Finally in section 5, conclusions and an outlook are presented.

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2. PROCESS MODEL

The process investigated in this work is the continuous production of poly acrylic acid (PAA) in a tubular reactor with multiple side feeds of monomer. The $P\&ID$ diagram of this reactor is shown in figure 1. The reactor comprises a total length of four meters and a volume of 720 ml. With the goal to reach efficient mixing of the reactants, the reactor has been equipped with static mixers. The reactor is divided into four zones where each two modules build a zone. The internal diameter of the modules of the first two zones is 12.1 mm whereas the other two zones have a diameter of 21 mm. At the nominal flow rate of 1 kg/hr, this configuration of the reactor leads to a total residence time of about 2600 seconds. The product quantity and quality are manipulated using the four side feeds of monomer (u_1, u_2, u_3, u_4) and the uniform jacket temperature of each zone of reactor $(T_{J1}, T_{J2}, T_{J3}, T_{J4})$. A measurement of the temperature in the middle of each zone of the reactor is available (T_1, T_2, T_3, T_4). A measurement of the viscosity at the reactor outlet is available and is used to compute the weight average molecular weight of the produced polymer (M_w). The residual monomer of the product is of interest for quality control and is represented by c_M in figure 1. This quantity is *not* measured.

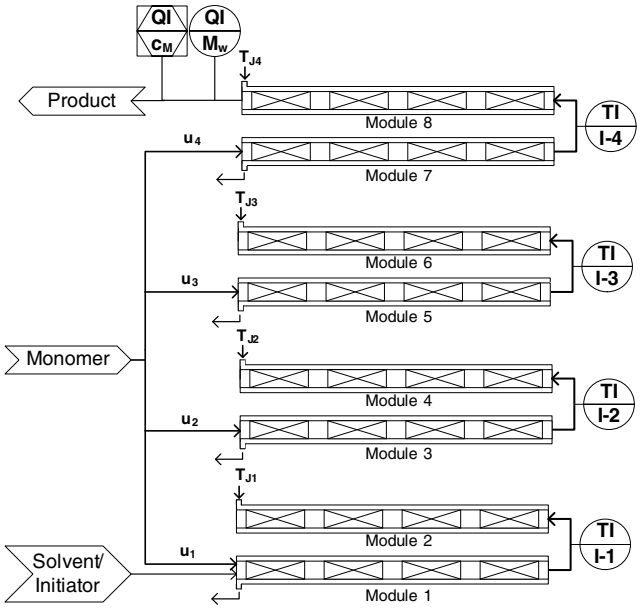

Fig. 1: Flow sheet of the modular continuous polymerization plant. (u_1, u_2, u_3, u_4): side feeds of monomer, $(T_{J1}, T_{J2}, T_{J3}, T_{J4})$: uniform jacket temperatures, M_w: weight average molecular weight (derived from a viscosity measurement), c_M: residual monomer of the product.

The simulation results presented in this work are based on a realistic model of this process. Assuming perfect mixing in the radial direction and using the energy and component balances for all components, a rigorous dynamic model for this process has been developed. The free radical polymerization of acrylic acid is modeled by the terminal model approach and the method of moments is used to model the polymer chain length distribution (Crowley et al. 1997). The reaction system is assumed to consist only of initiator decomposition, chain propagation and chain termination by combination. The resulting nonlinear partial differential equations (pde) are shown in equations 1 to 8 (Hashemi et al. 2016).

$$\frac{\partial c_I}{\partial t} = -u\frac{\partial c_I}{\partial z} + D_{ax}\frac{\partial^2 c_I}{\partial z^2} - k_d c_I \tag{1}$$

$$\frac{\partial c_M}{\partial t} = -u\frac{\partial c_M}{\partial z} + D_{ax}\frac{\partial^2 c_M}{\partial z^2} - k_p \lambda_0 c_M \tag{2}$$

$$\frac{\partial \lambda_0}{\partial t} = -u\frac{\partial \lambda_0}{\partial z} + D_{ax}\frac{\partial^2 \lambda_0}{\partial z^2} + 2fk_d c_I - 2k_{tr}{\lambda_0}^2 \tag{3}$$

$$\frac{\partial \lambda_1}{\partial t} = -u\frac{\partial \lambda_1}{\partial z} + 2fk_d c_I + k_p \lambda_0 c_M - k_{tr}\lambda_0\lambda_1 \tag{4}$$

$$\frac{\partial \lambda_2}{\partial t} = -u\frac{\partial \lambda_2}{\partial z} + 2fk_d c_I + k_p c_M\left(\lambda_0 + 2\lambda_1\right) - k_{tr}\lambda_0\lambda_2 \tag{5}$$

$$\frac{\partial \mu_1}{\partial t} = -u\frac{\partial \mu_1}{\partial z} + k_{tr}\lambda_0\lambda_1 \tag{6}$$

$$\frac{\partial \mu_2}{\partial t} = -u\frac{\partial \mu_2}{\partial z} + k_{tr}\lambda_0\lambda_2 + k_{tr}{\lambda_1}^2 \tag{7}$$

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial z} + \frac{\lambda}{\rho c_p}\frac{\partial^2 T}{\partial z^2} + \frac{Ak}{\rho c_p}\left(T_{jac} - T\right) + k_p\lambda_0 c_M\frac{-\Delta h_p}{\rho c_p} \tag{8}$$

where $z \in [0,\ 4]$ and denotes the spatial domain. c_I and c_M are the initiator and monomer concentrations respectively. λ_0, λ_1 and λ_2 represent the zeroth, first and second moment of active polymers. μ_1 μ_2 denote the first and second moment of inactive polymers and T is the reactor temperature. The temperature dependent rate coefficients k_d, k_p and k_{tc} are modeled using an Arrhenius approach. The weight average molecular weight of the product is computed from the moments as follows:

$$M_w = M_{\omega 0} \cdot \frac{\mu_2 + \lambda_2}{\mu_1 + \lambda_1}. \tag{9}$$

More details about the process model can be found in (Hashemi et al. 2016).

In this work, the *method of lines* is used to solve the pde model of the process. This means that the spatial derivatives of the pde model are substituted by algebraic approximations and therefore, the pde model is converted to an ode system which can be solved using the methods proposed for odes. The reactor system considered in this work reacts to the changes of the input flow rates with sharp concentration fronts and long settling times (figure 2). This is due to the near plug flow characteristic between the inputs and the outputs. In order to simulate such systems accurately, one possibility is to use low order finite differences schemes on very fine discretization grids to approximate the spatial derivatives of the pde model. However, such an approximation increases the size of the ode model drastically and therefore is impractical. Another possibility is to use so-called *high resolution methods* to approximate the spatial derivatives (Bouaswaig et al. 2009). We have used the *weighted essentially non-oscillatory scheme (WENO)* for this purpose and observed that a similar accuracy as for low order finite differences method can be achieved with a discretization grid which is 25 times smaller (Hashemi et al. 2016). For the details about the numerical method the reader is referred to (Borges et al. 2008) and (Liu et al. 2011). In this work, the spatial derivatives of the pde system are approximated using the WENO scheme on a discretization grid of 200 points which results in an ode model with 1600 states and this ode model is used throughout this paper. *CVODE* from the MATLAB interface of SUNDIALS has been used to simulate the model. A simulation of the this system is shown in figure 2.

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