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A Comparison of Nonlinear State Estimators for Closed-loop Control of Batch Crystallizers

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Abstract:
This study investigates the effectiveness of various nonlinear estimation techniques for output feedback model-based control of batch crystallization processes. Several nonlinear observers developed under deterministic and Bayesian estimation frameworks are applied for closed-loop control of a semi-industrial fed-batch crystallizer. The performance evaluation is done in terms of closed-loop behavior of the control strategy and its ability to cope with model imperfections and process uncertainties such as measurement errors and uncertain initial conditions. The simulation results suggest that the extended and the unscented Kalman filters perform best in terms of fulfilling the control objective. Adopting a time-varying process noise matrix, which is particularly suited for batch processes, further enhances the accuracy of state estimates at the expense of a slight increase in computational burden. The results also indicate that model imperfections and process uncertainties rather significantly deteriorate the closed-loop performance of the controller due to inaccurate state estimation.

Keywords: Batch crystallization; Moment model; Nonlinear model-based control; Observer; Kalman filters; Moving horizon estimator

1. INTRODUCTION

Batch crystallization is widely used in the pharmaceutical, food and fine chemical industries for the production of high value-added specialty chemicals. Model-based control of these processes in a closed-loop fashion typically requires knowledge of the system states. Despite the advent of process analytical technology in recent years (Braatz, 2002), on-line measurement of all process variables is not often viable due to various technological and economical limitations. The so-called state observers that combine information from two sources, namely a process model and available on-line measurements, can be utilized to estimate the states of a dynamic system in real time. Observers use measurement information to improve the quality of state estimates obtained by real-time simulation of the process model. This is done through a correction mechanism that essentially accounts for model imperfections and process uncertainties such as measurements errors and uncertain initial conditions.

Nonlinear observers can be broadly classified into two categories, namely the techniques developed under a deterministic framework and those developed under the Bayesian framework. While the deterministic observers neglect any noise acting on the system, the nonlinear observers developed under the Bayesian framework formulate the state estimation problem in a probabilistic setting. The estimation problem aims to construct probability density function (pdf) of the states, given that the process model and the measurements are subject to random disturbances.

The most widely used variant of the nonlinear stochastic observers is the extended Kalman filter (EKF). The EKF may result in significant estimation errors when the system is highly nonlinear or the state pdfs are non-Gaussian. In order to alleviate the shortcomings of the EKF, derivative free stochastic observers, namely the unscented Kalman filter (UKF) (Julier and Uhlmann, 2004) and Monte Carlo filters (Gordon et al., 1993) have been developed. While the state pdfs are assumed to be Gaussian, the UKF circumvents the need for computing the Jacobian matrices that may render the application of the EKF impractical for non-differentiable systems. On the other hand, Monte Carlo filters can handle nonlinear process dynamics without making any assumptions neither on the nature of the dynamics nor on the shape or any other characteristic of the pdfs. The estimation techniques developed under the Bayesian framework also include optimization-based observers. This approach enables explicit inclusion of constraints in the nonlinear estimation problem (Rawlings and Bakshi, 2006). In contrast to the stochastic observers, which make use of the most recent measurements, these estimators utilize measurements obtained over a certain time

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horizon to correct for the observation error. Optimization-based observers generally need not any assumption neither on the state pdfs nor on the noise sequences acting on the system.

This study is intended to investigate the effectiveness of several nonlinear observers for output feedback model-based control of industrial batch crystallizers. Successful implementation of a model-based control strategy largely relies on estimation accuracy of the current system states, which are utilized to make predictions of the process dynamics in future. The extended Luenberger observer and the extended Kalman filter are the most commonly used techniques for nonlinear state estimation in model-based control of batch crystallizers; see, e.g., Zhang and Rohani (2003) and Mesbah et al. (2008). Nonetheless, the shortcomings of these observers in coping with the highly nonlinear dynamics of crystallization systems that are subject to large process uncertainties necessitate the recourse to estimation techniques which better suit the inherent characteristics of batch crystallizers. Several state estimation techniques, including deterministic, stochastic and optimization-based techniques, are used to develop nonlinear observers for a semi-industrial seeded batch crystallizer. The dynamics of the process at hand are represented by a reduced-order moment model. The nonlinear observers are embedded in a model-based control framework. This facilitates comparative performance analysis of the observers in terms of their closed-loop control behavior as well as their ability to cope with model imperfections and process uncertainties. This paper aims to give an overview of the pros and cons of the aforementioned nonlinear estimation techniques when applied for on-line control of industrial batch crystallizers.

2. NONLINEAR STATE ESTIMATION TECHNIQUES

The class of nonlinear systems of interest is formulated in a discrete-time state space form

$$\begin{aligned} x_k &= f(x_{k-1}, u_{k-1}, w_{k-1}) \\ y_k &= h(x_k, u_k, v_k), \end{aligned} \tag{1}$$

where x_k is a vector of state variables, whose initial values are random variables with a given pdf; u_k is a vector of measured process inputs that are assumed to be constant over the time interval $[t_{k-1}, t_k]$; y_k is a vector of output measurements; $f(x_{k-1}, u_{k-1}, w_{k-1})$ is a nonlinear process model, which is generally the solution of a system of differential algebraic equations over the time interval $[t_{k-1}, t_k]$; $h(x_k, u_k, v_k)$ is a possibly nonlinear measurement model; w_k is a vector of process noise with $\mathbb{E}[w_k] = 0$ and $\mathbb{E}[w_k w_k^T] = Q_k$; v_k is a vector of measurement noise with $\mathbb{E}[v_k] = 0$ and $\mathbb{E}[v_k v_k^T] = R_k$. In the following, the algorithms of the nonlinear state estimation techniques considered in this work are presented.

2.1 Extended Luenberger Observer

For a deterministic system, i.e. $w = 0$ and $v = 0$, an extended Luenberger-type observer (ELO) (Zeitz, 1987) can be established as

$$\hat{x}_{k+1} = f(\hat{x}_k, u_k) + K_k(y_k - h(\hat{x}_k, u_k)), \tag{2}$$

where $\hat{x}_k$ is an estimate of the state vector and K_k is the observer gain that determines the convergence properties of the observer. The goal of the ELO is to provide an estimate of the state vector such that the observation error

$$\begin{aligned} e_{k+1} = x_{k+1} - \hat{x}_{k+1} = f(\hat{x}_k + e_k, u_k) - f(\hat{x}_k, u_k) - \\ K_k(h(\hat{x}_k + e_k, u_k) - h(\hat{x}_k, u_k)) \end{aligned} \tag{3}$$

is minimal. For nonlinear systems, a condition, under which the error converges to zero, cannot be readily deduced from the error dynamics. This implies that the observer gain needs to be determined on the basis of a linearized version of the original process model. Thus, linearizing the nonlinear model around $e = 0$ yields (Dochain, 2003)

$$e_{k+1} = (A_k - K_k C_k) e_k, \tag{4}$$

where $A_k = [\frac{\partial f(x_k, u_k)}{\partial x}]_{x_k = \hat{x}_k}$ and $C_k = [\frac{\partial h(x_k, u_k)}{\partial x}]_{x_k = \hat{x}_k}$ are linear approximations of the nonlinear process dynamics around the estimated state vector $\hat{x}_k$. The choice of the observer gain K_k relies on local stability properties of the state estimator. The gain should be chosen such that the linearized error dynamics are asymptotically stable.

In general, the estimation accuracy of the ELO largely depends on how well the linearized model represents the nonlinear process dynamics. Initialization of the observer is also crucial since accurate linearization of process and measurement functions around $e = 0$ requires that the observer is initialized sufficiently close to the true states.

2.2 Extended Kalman Filter

The extended Kalman filter, which is founded on the notion presented by Kalman and Bucy (1961) for linear systems, is the most widely used state estimation technique in diverse process control applications. This is due to its relatively easy implementation and limited computational burden (Soroush, 1998). The EKF requires that the initial state variables x_0 and the noise sequences acting on the system, i.e. w and v, to be random variables with Gaussian distributions. The latter pdfs however remain no longer Gaussian once undergone through nonlinear transformations. Hence, the EKF presents a suboptimal solution to the state estimation problem of nonlinear systems since it assumes that the random variables still retain their Gaussian distribution after the transformation.

The EKF has a recursive algorithm consisting of two parts, namely the prediction stage and the measurement correction stage. In the former stage, the a priori state estimates $\hat{x}_{k+1|k}$ and their associated error $P_{k+1|k}$ are determined by propagating the mean $\hat{x}_{k|k}$ and covariance $P_{k|k}$ of the state pdfs at the preceding time step through the nonlinear process model and its first order linearization, respectively,

$$\begin{aligned} \hat{x}_{k+1|k} &= f(\hat{x}_{k|k}, u_k, w_k) \\ P_{k+1|k} &= F_k P_{k|k} F_k^T + W_k Q_k W_k^T, \end{aligned} \tag{5}$$

where $F_k = [\frac{\partial f(x_k, u_k, w_k)}{\partial x}]_{x_k = \hat{x}_{k|k}}$ and $W_k = [\frac{\partial f(x_k, u_k, w_k)}{\partial w}]$. Subsequently, in the measurement correction stage the a posteriori state estimates $\hat{x}_{k+1|k+1}$ and their error $P_{k+1|k+1}$ are calculated using current measurements y_k

$$\begin{aligned} \hat{x}_{k+1|k+1} &= \hat{x}_{k+1|k} + K_k(y_k - h(\hat{x}_{k+1|k}, u_k, v_k)) \\ P_{k+1|k+1} &= (I - K_k H_k) P_{k+1|k}. \end{aligned} \tag{6}$$

K_k is the Kalman filter gain defined as

$$K_k = P_{k+1|k} H_k^T (H_k P_{k+1|k} H_k^T + V_k R_k V_k^T)^{-1}, \tag{7}$$

where $H_k = [\frac{\partial h(x_k,u_k,v_k)}{\partial x}]_{x_k=\hat{x}_{k+1|k}}$ and $V_k = [\frac{\partial h(x_k,u_k,v_k)}{\partial v}]$.

Despite its extensive use, the EKF suffers from several practical shortcomings, namely its inapplicability to highly nonlinear, non-differentiable systems, difficult tuning and inability to systematically incorporate state constraints. A critical evaluation of the extended Kalman filter is given in (Wilson et al., 1998), where the authors have raised their serious doubts on the usefulness of the EKF in industrial applications.

2.3 Unscented Kalman Filter

The unscented Kalman filter is primarily developed to alleviate the main deficiency of the EKF, i.e. linear approximation of the nonlinearities, by applying the unscented transformation to the Kalman estimation notion. According to Julier and Uhlmann (2004), the underlying idea is to approximate the Gaussian pdf of the states by a number of deterministically chosen points, the so-called sigma points, such that their mean and covariance match those of the prior distribution. These points are then propagated through the nonlinear system model to determine expectations and covariances of the state estimates. Clearly, this is in contrast to the EKF that propagates only a single point through a linearized version of the original system model.

The filter algorithm is defined on the basis of the same steps as in the EKF. A set of $2n + 1$ symmetric sigma points, where n denotes the dimension of the state vector, is generated around the means of the set with a distance of the square root of the covariances. Once the sigma points are chosen, they are propagated through the nonlinear model equations to calculate the predicted mean and covariance based on the transformed set of points

$$\begin{aligned} \chi^i_{k+1} &= f(\chi^i_k, u_k, w_k) \\ P_{k+1|k} &= \sum_{i=1}^{2n+1} W_i[\chi^i_{k+1} - \hat{x}_{k+1|k}][\chi^i_{k+1} - \hat{x}_{k+1|k}]^T \\ \hat{x}_{k+1|k} &= \sum_{i=1}^{2n+1} W_i \chi^i_{k+1}. \end{aligned} \tag{8}$$

It is evident that the prediction stage differs from the EKF in that the unscented Kalman filter does not linearize the nonlinear model. Instead, it propagates a cluster of points, centered around the current state estimates, to more accurately approximate mean and covariance of the state pdfs. The a priori state vector and its associated covariance are then updated using measurements y_k

$$\begin{aligned} \gamma^i_{k+1} &= h(\chi^i_k, u_k, v_k) \\ \hat{y}_{k+1|k} &= \sum_{i=1}^{2n+1} W_i \gamma^i_{k+1} \\ P_{yy,k+1|k} &= \sum_{i=1}^{2n+1} W_i[\gamma^i_{k+1} - \hat{y}_{k+1|k}][\gamma^i_{k+1} - \hat{y}_{k+1|k}]^T \\ P_{xy,k+1|k} &= \sum_{i=1}^{2n+1} W_i[\chi^i_{k+1} - \hat{x}_{k+1|k}][\gamma^i_{k+1} - \hat{y}_{k+1|k}]^T \\ K_k &= P_{xy,k+1|k} P^{-1}_{yy,k+1|k} \\ \hat{x}_{k+1|k+1} &= \hat{x}_{k+1|k} + K_k(y_k - \hat{y}_{k+1|k}) \\ P_{k+1|k+1} &= P_{k+1|k} - K_k P_{yy,k+1|k} K^T_k, \end{aligned} \tag{9}$$

where W_i denote the weighting coefficients.

The computational efficiency of the UKF is comparable to that of the EKF; being in the order of $O(n^3)$ operations, provided that the dimension of the state vector is large compared to the number of measurements. The UKF is however easier to implement and provides at least second order accuracy for the covariance approximations, while the EKF is only accurate up to the first order moment of the pdfs.

2.4 Ensemble Kalman Filter

The ensemble Kalman filter (EnKF) (Evensen, 1997), belonging to the broader class of Monte Carlo filters, constitutes a class of derivative free nonlinear filters that can cope with multimodal and non-Gaussian distributions. The EnKF is a suboptimal estimator, where the error statistics are predicted by solving the Fokker-Planck equation by means of a Monte Carlo method. The underlying notion of the EnKF is to represent the state pdfs by a large ensemble of randomly chosen states, which aims to describe all statistical properties of the system variables. Integrating the ensemble members forward in time according to the stochastic system dynamics is equivalent to solving the Fokker-Planck equation using a Monte Carlo method.

In the prediction stage of the filter algorithm, a set of sample points, i.e. $\hat{x}^i_{k|k}$, that describes the statistics of the state pdfs is generated using the Monte Carlo sampling. The sample points are propagated through the nonlinear system to compute a cloud of transformed sample points

$$\hat{x}^i_{k+1|k} = f(\hat{x}^i_{k|k}, u_k, w_k). \tag{10}$$

These sample points are then used to estimate the a priori sample mean and error covariance matrices

$$\begin{aligned} \bar{x}_{k+1|k} &= \frac{1}{N}\sum_{i=1}^{N} \hat{x}^i_{k+1|k} \\ \bar{y}_{k+1|k} &= \frac{1}{N}\sum_{i=1}^{N} h(\hat{x}^i_{k+1|k}, u_k, v_k) \\ E_{x_{k+1|k}} &= [\hat{x}^1_{k+1|k} - \bar{x}_{k+1|k} \quad \cdots \quad \hat{x}^N_{k+1|k} - \bar{x}_{k+1|k}] \\ E_{y_{k+1|k}} &= [\hat{y}^1_{k+1|k} - \bar{y}_{k+1|k} \quad \cdots \quad \hat{y}^N_{k+1|k} - \bar{y}_{k+1|k}] \\ P_{xy,k+1|k} &= \frac{1}{N-1} E_{x_{k+1|k}} E^T_{y_{k+1|k}} \\ P_{yy,k+1|k} &= \frac{1}{N-1} E_{y_{k+1|k}} E^T_{y_{k+1|k}}. \end{aligned} \tag{11}$$

The error covariance matrices are defined around the ensemble mean, implying that the ensemble mean provides the best estimate of the state variable and the spread of the ensemble members around the mean is a natural definition of the error of the ensemble mean. Finally, the EnKF performs an ensemble of parallel data assimilation steps to obtain the a posteriori state estimates

$$\begin{aligned} K_k &= P_{xy,k+1|k} P^{-1}_{yy,k+1|k} \\ \hat{x}^i_{k+1|k+1} &= \hat{x}^i_{k+1|k} + K_k(y_k - h(\hat{x}^i_{k+1|k}, u_k, v_k)) \\ \bar{x}_{k+1|k+1} &= \frac{1}{N}\sum_{i=1}^{N} \hat{x}^i_{k+1|k+1}. \end{aligned} \tag{12}$$

The computational cost of the EnKF is in the order of $O(pNn)$ operations, where p is the number of outputs of the system, N is the ensemble size and n is the dimension of the state vector (Gillijns et al., 2006). Thus, if $N << n$, the computational burden of the EnKF will be less than that of the EKF. When N is large, the EnKF will however become computationally too expensive since the model needs to be simulated N times.

2.5 Moving Horizon Estimator

What distinguishes the moving horizon estimator from other estimation techniques is its ability to incorporate constraints in the estimation problem. The MHE is an optimization-based estimator, wherein the state estimates are obtained by solving a minimization problem such as the sum of squared errors (Robertson et al., 1996). On the contrary to the classical state estimators, which only utilize the most recent measurements to update the model predictions, the MHE uses measurements gathered over a certain time interval for the observer correction.

The moving horizon estimation problem can be stated in its most general form as the solution of the following optimization problem (Rao and Rawlings, 2002)

$$\min_{x_{T-P},\{w_k\}_{k=T-P}^{T-1}} \sum_{k=T-P}^{T-1} ||v_k||^2_{R^{-1}} + ||w_k||^2_{Q^{-1}} + Z_{T-P}(x_{T-P}) \tag{13}$$

$$\text{subject to}: \quad \text{equation (1)}$$
$$x_k \in X, w_k \in W, v_k \in V,$$

where the sets X, W and V can be constrained; P is the horizon size. Equation (13) implies that the last P measurements are explicitly used to solve the optimal estimation problem over time horizon $T-P \leq k \leq T-1$. The remaining process measurements are accounted for by using function $Z_{T-P}(x_{T-P})$, the so-called arrival cost term, which essentially summarizes the effect of the prior measurement information on the state estimates at time instant $T-P$. In fact by providing a means to compress data, the arrival cost term facilitates the transformation of an infinite dimensional optimization problem into one of finite dimension. Exact algebraic expressions for the arrival cost term only exist for unconstrained, linear systems under Gaussian assumptions, where the moving horizon estimator reduces to the Kalman filter. In the case of constrained, nonlinear systems the arrival cost term needs to be approximated in order to compute the error covariance of the estimated states at time instant $T-P$. Adequate approximation of the arrival cost term is crucial to guaranteeing stability and performance of the MHE.

3. CASE STUDY: A SEMI-INDUSTRIAL FED-BATCH CRYSTALLIZER

The above discussed estimation techniques are used to design nonlinear observers for seeded fed-batch evaporative crystallization of an ammonium sulphate-water system. The crystallization tales place in a semi-industrial crystallizer. In general, the nonlinear dynamics of crystallization systems are described by a set of differential algebraic equations

$$\begin{aligned} \dot{x} &= f(t,x,z,y,u,\theta) \qquad x(t_0) = x_0 \\ 0 &= g(t,x,z,y,u,\theta) \\ y &= h(t,x,z,y,u,\theta), \end{aligned} \tag{14}$$

Table 1. Computational times of the observers

Nonlinear observer	Average CPU-time * of one iteration, s
ELO	0.012
EKF	0.012
EKF (Time-varying Q)	0.013
UKF	0.032
UKF (Time-varying Q)	0.033
EnKF	0.157
MHE	0.424

* The reported CPU-times correspond to the Microsoft Windows XP (Professional) operating system running on a Genuine Intel(R) T2050 @1.60GHz processor with 1 GB RAM.

where f, g and h are the sets of explicit system state, algebraic and output equations, respectively; t is the time; x is the state vector; z is the vector of algebraic variables; y is the vector of measurements; u is the vector of process inputs; θ is the model parameter set. For the system at hand, the state vector contains the five leading moments of crystal size distribution (CSD) and the solute concentration, whereas the vector of algebraic variables consists of kinetic variables, namely total nucleation and crystal growth rates. As the evolution of CSD throughout a batch run is measured, the five leading moments of CSD comprise the output vector. On the other hand, heat input to the crystallizer serves as the only mechanism to generate supersaturation and consequently govern the crystallization process. Note that in equation (14) x_0 represents the initial states of the system determined by the seed characteristics and the initial solute concentration. A detailed description of the fed-batch crystallizer under study and its nonlinear process model can be found in (Mesbah et al., 2009).

In order to assess the performance of the nonlinear estimation techniques for on-line closed-loop control of the crystallizer, the observers are embedded in an output feedback model-based control framework; see Fig. (1). As discussed in (Mesbah et al., 2008), the observer plays a key role in this control strategy through estimating the states of the system at each sampling time interval when measurements y_{meas} become available. The estimated states $\hat{x}$ are used to recursively initialize the dynamic optimizer, which calculates the optimal operating policy of the crystallizer, i.e. u_{opt}, such that a maximum admissible crystal growth rate is maintained throughout a batch run. In this study, the model-based control strategy is applied to a plant simulator that simulates the system by using exactly the

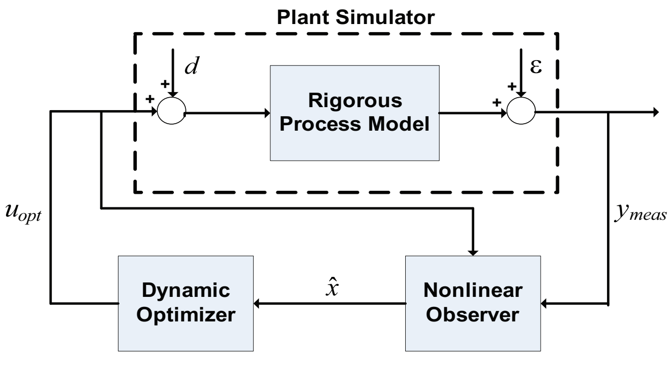

Fig. 1. Output feedback model-based control framework.

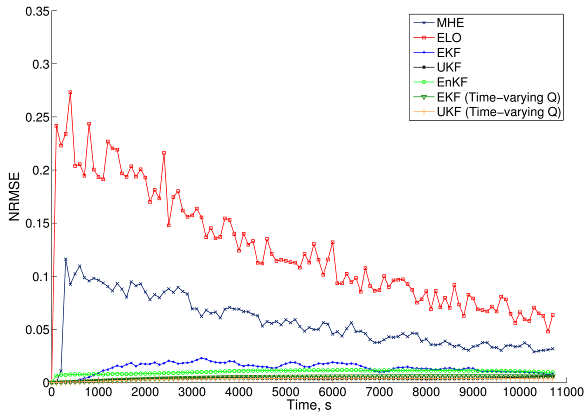

Fig. 2. Estimation errors of the 2^{nd} moment of CSD under the nominal scenario.

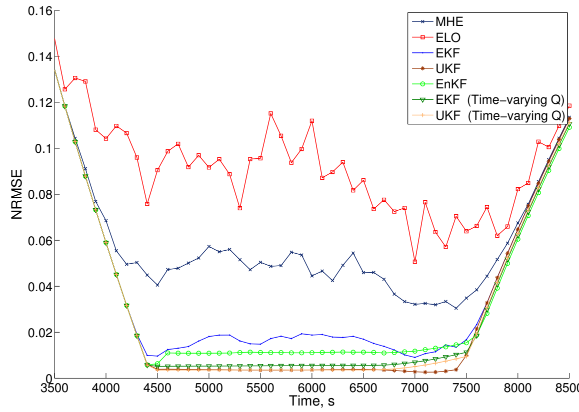

Fig. 3. Errors in the reference crystal growth rate trajectory tracking under the nominal scenario.

same nonlinear process model as the one incorporated in the observer and the dynamic optimizer. The closed-loop performance of the control strategy, which is largely dependent on the quality of state estimates, is evaluated under the following scenarios:

- nominal case, where the measurements are corrupted by random noise sequences possessing normal distributions;
- uncertain case, which aims to examine how well the control objective, namely the reference crystal growth rate trajectory tracking, is fulfilled in the presence of model imperfections and process uncertainties.

The tuning parameters of the observers remain fixed under the two scenarios in order to have a fair performance evaluation. The errors associated with the estimated states are expressed in terms of the normalized root mean squared error (NRMSE)

$$\mathtt{NRMSE} = \sqrt{\mathbb{E}\big[\big(\frac{x(t)-\hat{x}(t)}{x(t)}\big)^2\big]}, \tag{15}$$

where the expected value of the relative estimation errors is defined on the basis of 50 simulation runs.

Fig. (2) shows the estimation errors of the 2^{nd} moment of CSD for all nonlinear observers under the nominal scenario. Amongst the five leading moments of CSD, the control objective, which is calculated on the basis of the solute concentration estimates, is more closely related to the 2^{nd} moment. As can be seen, the ELO exhibits the worst estimation accuracy, whereas the other observers, in particular the EKF and the UKF, provide state estimates with considerably less errors. This is attributed to the inability of the ELO to effectively cope with measurement noise due to its deterministic estimation framework. In order to further improve the quality of state estimates obtained by the EKF and the UKF, a time-varying process noise matrix that particularly suits batch processes is adopted (Valappil and Georgakis, 2000). Fig. (2) suggests that the latter tuning approach results in a better estimation quality. As shown in Table (1), the additional computational effort required for computing the time-varying process noise matrix is small.

The extent to which the estimation quality of states influences the effectiveness of the model-based control strategy in terms of the reference crystal growth rate trajectory tracking is investigated. Fig. (3) shows the normalized root mean squared errors of the control objective. The errors are calculated on the basis of deviations of the crystal growth rate with respect to its reference trajectory in the time frame over which the control objective can be fulfilled. As can be seen, the relatively poor state estimation by the ELO and the MHE leads to ineffective fulfillment of the maximum admissible crystal growth rate. On the other hand, as expected, the Kalman filters allow the controller to more closely track the reference trajectory that in turn will result in a product with the desired quality attributes. The increase in estimation errors at approximately 7500 s is due to the inability of the controller to closely follow the reference trajectory at all times during a batch run.

The capacity of the nonlinear observers in coping with model imperfections and process uncertainties is investigated under the uncertain scenario. The kinetic parameters of the underlying model of the control strategy are varied for 35% with respect to their nominal values in the plant simulator. Process uncertainties are induced through uncertain initial conditions and systematic measurement

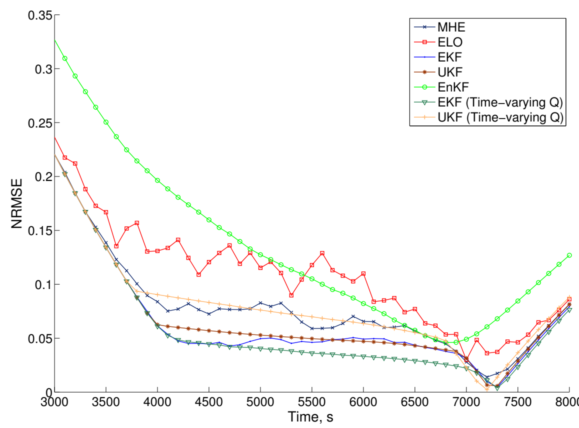

Fig. 4. Errors in the reference crystal growth rate trajectory tracking under the uncertain scenario.

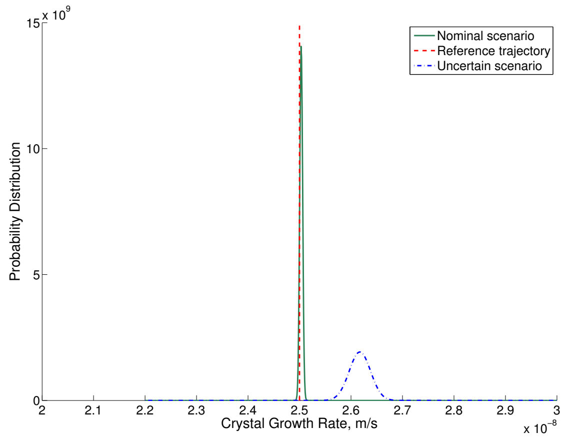

Fig. 5. Normal probability distribution of the crystal growth rates estimated by the UKF.

errors. The five leading moments of CSD and the solute concentration used to initialze the controler's model are varied for 5% and 2%, respectively, with respect to their nominal values. Alongside the stochastic noise, the process measurements, i.e. the moments of CSD, are corrupted by a 5% off-set with rescpect to the actual model outputs. As shown in Fig. (4), the model-based controller fails to tightly follow the reference trajectory. The process uncertainties lead to a rather significant deviation of the crystal growth rate from its reference trajectory. This is due to the inability of the observers to effectively deal with systematic measurement errors and uncertain initial conditions. A remedy for this problem is the inclusion of augmented states in order to effectively account for the off-set in the closed-loop control performance. Fig. (5) depicts the normal probability distribution of the crystal growth rate estimated by the UKF under both scenarios; the dashed line represents the maximum admissible crystal growth rate. It is well-evident that the crystal growth rates infered under the uncertain scenario exhibit a rather large off-set with respect to the reference trajectory. This may considerably degrade the product quality. On the other hand, the effectiveness of the EKF and the UKF in providing accurate state estimates under the nominal scenario enables the controller to achieve its objective fairly well.

4. CONCLUSIONS

Several nonlinear observers developed under deterministic and Bayesian estimation frameworks have been applied for output feedback model-based control of a semi-industrial fed-batch crystallizer. The simulation results indicate that the state estimates provided by the ELO and the MHE in the presence of stochastic measurement noise are of somewhat worse quality than those made by the Kalman filters, whose estimation ability can even be further enhanced by adopting a time-varying process noise matrix. This is due to the deterministic estimation framework of the ELO and the elimination of the arrival cost term in the MHE that in fact reduces its Bayesian framework to a deterministic optimization-based estimation technique. The simulation results also suggest that the model-based controller fails to adequately fulfill its objective in the presence of model imperfections and process uncertainties due to the inability of the nonlinear observers to provide accurate state estimates.

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