Stochastic Nonlinear Observers for Industrial Seeded Batch Crystallization Processes

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A substantial amount of materials in the pharmaceutical, food, and fine chemical industry is produced in crystalline form. Batch crystallization is a key separation and purification unit in such industries, with a significant impact on the efficiency and profitability of the overall process. Advanced model-based control of crystallization processes offers many possibilities to achieve the stringent requirements of the final product quality, such as crystal size, purity and morphology, and also enhance the process efficiency.

The control of batch crystallization processes is traditionally done by tracking predetermined batch recipes using PID controllers. As the recipes are largely based on operator's experience, they often lack the ability to systematically push the process to its most optimal operating trajectory while various operational and quality limitations are met.

In the recent years, the development of computationally powerful modeling and optimization tools has considerably facilitated the use of first principle models in devising optimal batch recipes. Application of the off-line optimization approach is however insufficient as plant-model mismatch, process disturbances and uncertain initial conditions often deteriorate the effectiveness of the off-line optimized operating policies. A remedy for the latter deficiency is real-time optimal control of the batch process in a receding horizon framework [1][2]. The closed-loop optimal control approach continuously optimizes the system in the presence of plant-model mismatch and unmeasured disturbances and, therefore, drives the process to its most optimal operation at any time during the batch. The effectiveness of this model-based control strategy is due to the feedback of measurements that are used by an observer to estimate the system states. The observer essentially facilitates implementation of the receding horizon framework that makes the control strategy less sensitive to process disturbances and variations. Furthermore, the observer enables the estimation, i.e. soft sensing, of process variables, for which actual measurements may not be available due to various technological and economical limitations.

Observers enable estimation of the state variables based on a process model, as well as in-situ measurements. The design of observers for batch crystallization processes is a challenging task due to a variety of reasons. These processes are distributed systems typically represented by a set of differential algebraic equations; derived from the population balance equation using discretization schemes. The complexity of the process model arisen from the large number of differential equations, which are often highly nonlinear due to the complex kinetic expressions, necessitates efficient observation techniques to render real-time implementation of the control strategy computationally feasible. More importantly, the intrinsic characteristics of batch crystallization processes, namely unmeasured disturbances and uncertain initial conditions due to improper seeding, as well as practical deficiencies such as plant-model mismatch and measurement errors often degrade the performance of the control strategy. In the measurement feedback framework, the observer should therefore be able to account for performance degradation of the model-based controller arisen form the afromentioned sources of error.

In this work, three extensions of the Kalman filter, namely the Extended Kalman Filter (EKF), the Ensemble Kalman Filter (EnKF) [3] and the Unscented Kalman Filter (UKF) [4], have been thoroughly investigated to design an observer best suited for batch crystallization processes.

These filtering techniques have the capacity not only to efficiently handle systems with nonlinear dynamics but also coping effectively with stochastic disturbances and measurement errors in the processes under study. In these variants of the Kalman filter, the state variables are represented by Gaussian Random Variables (GRV) that are then propagated through the system model. In the EKF, the system dynamics are linearized around the mean of the GRV. On the contrary, the random variables are approximated by a number of points chosen deterministically and stochastically in the UKF and EnKF respectively, which are transformed through the nonlinear system. Besides their higher estimation accuracy, the latter filters are expected to better suit highly nonlinear, non-differentiable systems.

In order to assess the performance of the filters, a semi-industrial 75-liter fed-batch crystallizer has been taken as a benchmark; the process at hand is adequately represented by a moment model consisting of the first five leading moments of the crystal size distribution and the solute concentration balance. The performance of the filters has been evaluated in the closed-loop mode in terms of their estimation accuracy and computational burden. In various tests, the effect of different sources of error on performance deterioration of the model-based control strategy due to poor state estimation has also been investigated.

The results of this study clearly indicate the importance of assessing various characteristics of an observation technique in the receding horizon framework when the observer is to be designed for a real-time model-based control application. The simulation results reveal that all three filters exhibit almost the same estimation accuracy, though the EnKF has a somewhat higher computational burden in the closed-loop mode. Fairly smooth state profiles are however obtained using the EnKF as its tuning can be done more easily than the other filters. Furthermore, the closed-loop tests show that in the presence of plant-model mismatch and uncertain initial conditions all the filtering techniques fail to satisfactorily fulfill the control objective, which is to follow a predetermined growth rate reference trajectory. This necessitates the addition of extra system states, the so-called augmented states, in order to restore the effectiveness of the control strategy. The augmented states enable us to account for biased state estimations in the observer. This issue is currently being investigated.

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