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A comparison of nonlinear observers for output feedback model-based control of seeded batch crystallization processes

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ABSTRACT

This paper presents a comparative analysis of various nonlinear estimation techniques when applied for output feedback model-based control of batch crystallization processes. Several nonlinear observers, namely an extended Luenberger observer, an extended Kalman filter, an unscented Kalman filter, an ensemble Kalman filer and a moving horizon estimator are used for closed-loop control of a semi-industrial fed-batch crystallizer. The performance of the nonlinear observers is evaluated in terms of their closed-loop behavior as well as their ability to cope with model imperfections and process uncertainties such as measurement errors and uncertain initial conditions. The simulation results suggest that the extended Kalman filter and the unscented Kalman filter provide accurate state estimates that ensure adequate fulfillment of the control objective. The results also confirm that adopting a time-varying process noise covariance matrix further enhances the estimation accuracy of the latter observers at the expense of a slight increase in their computational burden. This tuning method is particularly suited for batch processes as the state variables often vary significantly along the batch run. It is observed that model imperfections and process uncertainties are largely detrimental to the accuracy of state estimates. The degradation in the closed-loop control performance arisen from inadequate state estimation is effectively suppressed by the inclusion of a disturbance model into the observers.

1. Introduction

Batch crystallization is extensively utilized in the pharmaceutical, food and fine chemical industries for the production of high value-added specialty chemicals. Model-based control and performance monitoring of these processes typically require knowledge of the system states. In most crystallization applications, measurements of crystal size distribution (CSD) and solute concentration, along with temperature, are essential. Despite the advent of process analytical technology in recent years [7], online measurement of all process variables is not often viable due to various technological and economical limitations. Several challenges yet exist in reliable measurement of the evolution of CSD and solute concentration during a batch crystallization process. The merits and demerits of online sensors commonly utilized for measuring CSD and solute concentration have been extensively investigated in the literature; see, e.g. [50,30] and the references therein.

In theory, the unmeasurable process variables can be estimated by real time simulation of a crystallization model in parallel to the process. However, process models typically exhibit structural and parametric mismatch with respect to the real process. The model imperfections, alongside uncertain initial conditions, unmeasured process disturbances and measurement errors, tend to degrade the quality of the estimated process variables. A remedy for this deficiency is the use of state observers that combine information from two sources, namely a process model and available online measurements, to estimate the states of a dynamic system in real time.

A wide variety of approaches for state estimation of nonlinear dynamic systems have been proposed in the literature. The nonlinear state observers commonly used in (bio)chemical process applications can be categorized into exponential and asymptotic estimation techniques [3]. The former class of observers assumes a perfect knowledge of the model structure including the process kinetics, whereas the asymptotic observers merely rely on conservation laws without requiring the knowledge of process kinetics. Thus, the great deal of uncertainty associated with the kinetic parameters is eliminated in the asymptotic observers. However, this is achieved at the expense of a convergence rate that is fully governed by the process conditions, while the adjustable rate of convergence of the exponential observers is determined by tuning parameters [15]. To overcome the shortcomings of these estima-

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