Chapter 32
Modeling and Monitoring of Chemical System: CSTR Model

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ABSTRACT

This chapter addresses the problem of time-varying nonlinear modeling and monitoring of a continuously stirred tank reactor (CSTR) process using state estimation techniques. These techniques include the extended Kalman filter (EKF), particle filter (PF), and the more recently the variational Bayesian filter (VBF). The objectives of this chapter are threefold. The first objective is to use the variational Bayesian filter with better proposal distribution for nonlinear states and parameters estimation. The second objective is to extend the state and parameter estimation techniques to better handle nonlinear and non-Gaussian processes without a priori state information, by utilizing a time-varying assumption of statistical parameters. The third objective is to apply the state estimation techniques EKF, PF and VBF for time-varying nonlinear modeling and monitoring of CSTR process. The estimation performance is evaluated on a synthetic example in terms of estimation accuracy, root mean square error and execution times.

INTRODUCTION

Many process operations, such as modeling, monitoring, and control, require the availability of key process variables or parameters that are essential for the effective implementation of these operations. In some cases, however, measuring or estimating these variables or parameters might be practically difficult or costly. For example, it is challenging to accurately measure the concentrations inside a reactor or the compositions in a distillation column online, which are needed to control and/or monitor these processes.

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In such cases, state estimation techniques are usually used to estimate the sought variables (called state variables) online from measurements of other variables(s). State estimation techniques can also be used to model various processes. For example, deriving dynamic models of chemical reactors can be achieved using material and energy balances. However, such models contain several parameters (such as the reaction rate constant, reaction order, heat transfer coefficient, heat of reaction, and others) that may not be known. Determining these parameters usually requires several experimental setups that can be challenging and expensive in practice. Estimating these parameters using state estimation techniques can be of a great value. In this chapter, state estimation will be utilized to model and monitor a continuously stirred tank reactor (CSTR) by estimating its model parameters and state variables (concentration and temperature inside the reactor), respectively. A comparative analysis involving various conventional as well as state-of the-art state estimation techniques will be performed to achieve this objective.

The contributions of this chapter are four-fold. The first contribution is to develop a variational Bayesian filter algorithm for nonlinear and non-Gaussian estimation. In case of standard PF, the latest observation is not considered for the evaluation of the weights of the particles as the importance function is taken to be equal to the prior density function. The second contribution is to extend the state and parameter estimation techniques (i.e., EKF, PF, and VBF) to better handle nonlinear and non-Gaussian processes without a priori state information, by utilizing a time-varying assumption of statistical parameters. The third contribution of this chapter is to investigate the effects of practical challenges on the performances of the EKF, PF, and VBF algorithms. The comparative analysis is conducted to study the effect of the number of states and parameters to be estimated on the estimation performances of various estimation techniques: EKF, PF, and VBF. Similarly, to investigate the effect of measurement noise on the estimation performances, several measurement noise contributions (e.g., different signal-to-noise ratios) will be considered. Then, the estimation performances of EKF, PF, and VBF will be compared for different noise levels. Also, to study the effect of the number of states and parameters to be estimated on the estimation performances of EKF, PF, and VBF, the estimation performance will be analyzed for different numbers of estimated states and parameters. The fourth contribution of this chapter is to apply the estimation techniques (EKF, PF, and VBF) to estimate the states and parameters of a chemical model representing the CSTR process.

The rest of the chapter is organized as follows. We first discuss related works and motivate the need for our proposed work in Section II. In Section III, a statement of the problem addressed in this chapter is presented. In Section IV, a description of variational Bayesian filter is presented. Then, in Section V, the performances of the various state estimation techniques are compared through their application to estimate the state variables and model parameters of a CSTR process. Finally, some concluding remarks are presented in Section VI.

RELATED WORKS

Several state estimation techniques have been developed and used to achieve this objective. These techniques include the extended Kalman filter (EKF) (Lillacci & Khammash, 2010), the unscented Kalman filter (UKF) (Gustafsson & Hendeby, 2012), the particle filter (PF) (Arulampalam et al., 2005), and more recently the variational Bayesian filter (VBF) (Mansouri et al., 2014). The classical Kalman Filter (KF) was developed in the 1960s (Kalman, 1960), and has been widely applied in various engineering