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Design of a dynamical hybrid observer for pressure swing adsorption processes

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ABSTRACT

As an integral part of a hybrid control system for Pressure Swing Adsorption (PSA) processes, a dynamical hybrid observer is proposed for online reconstruction of the active mode and continuous states of these processes. Hybrid systems feature both continuous and discrete-event dynamics and hence are very suited to describe PSA processes. For estimation of the active mode, a mode observer is designed, and the continuous spatial profiles in each mode are estimated by distributed and decentralized Kalman filters. The proposed hybrid observer has been applied, in silico, for a two-bed, six-step PSA process used for Hydrogen purification. The active mode of the process along with the continuous spatial profiles of its adsorption beds have been estimated quite accurately based on the measured temperatures and pressures at a few points in the process, these measured signals are all noise-corrupted and measured discretely.

Introduction

Pressure Swing Adsorption (PSA) is a well-known and widely-used technology for separation and purification of gas mixtures [1–3]. PSA processes are autonomous distributed parameter switching systems with fix mode sequences. During the switching modes of the process, separation of gas species is performed by cyclic adsorption and desorption at higher and lower operating pressures. In modern industrial PSA systems, simple proportional controllers are used for regulation of the switch times, especially the adsorption time, based on the flow rate and temperature of feed stream. Recently, the control of PSA processes attracted more interest, although a few studies were reported in the literature [4–8] which are focused on regulation of switching times of PSA systems mainly based on the estimated product purity of the process. Product purity is the main decision variable in PSA processes and having the concentration profile is significant; however, its measurement requires large sampling time and is available only at the end of adsorption beds. Moreover, the number of pressure and temperature measurements is very limited in PSA processes. This leads to one of the most important challenges in the use of Advanced Process Control (APC) methods for these processes, due to the loss of information corresponding to the spatial profiles along the adsorption beds. On the other hand, an accurate knowledge of active mode of the operation is necessary to achieve an

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appropriate mode transition scenario based on an efficient control strategy. Hence, design of a hybrid observer for the reconstruction of both modes and continuous states of the process is an utmost necessity for efficient control and monitoring of the PSA processes. The mode observer is a Discrete Event System (DES) model of the process that identifies the active mode based on the available continuous measurements from the PSA process. Once the active mode is known, a proper continuous observer can efficiently estimate the profiles of pressure, temperature, and concentration in particular.

Design of continuous state observer for adsorption systems was the topic of a few studies [9–13]. Mangold et al. [9] proposed an observer based on a simplified linear distributed parameter model of an adsorption bed. The observer states were corrected based on physical and heuristic considerations. Yang et al. [10] designed an extended Kalman Filter based on a linear low-order model for breakthrough estimation using temperature measurements in an ion-exchange adsorption column. Bitzer and Zeitz [11] used a nonlinear distributed parameter observer for estimation of spatial profiles of a PSA process. Their observer follows Luenberger's idea and the observer gain was calculated intuitively instead of obtaining through solving Riccati equation. Won and Lee [12] presented a nonlinear observer with adaptive grid allocation to estimate the spatial profiles in adsorption stage of an adsorption bed in the presence of measurement noise. They have used a simplified Kalman filter in which its observer gain is a static function of the state variables to overcome the time-consuming procedure of standard Kalman filter.

The hybrid nature of the PSA process was never considered in the aforementioned works. In the previous work by Fakhroleslam et al. [13] a Distributed and Decentralized Switching Kalman Filter (DDSKF) was designed for estimation of spatial profiles in PSA processes, assuming that the active mode of the process is known. A Reduced Order Model (ROM) of the process was obtained by Orthogonal Collocation Method (OCM) and the pressure and temperature sensors were optimally located. The spatial profiles of the system were estimated based on noise-corrupted measured temperature and pressure of a few points in the process.

In this work, the assumption of knowing the active mode in Ref. [13] is relaxed and the focus is on the design of a *mode observer*, which is also known as *location observer* in some literature [14–16]. This mode observer along with the introduced continuous observer DDSKF is an integral part of a hybrid observer designed for PSA processes. The design of mode observer for PSA processes has not been studied in the literature yet. The design of hybrid observers was the topic of several studies in the literature [15–23], some of which have focused on design of mode observers [15,17–19]. Fliess et al. [17] studied the distinguishability of linear switching systems and proposed a mode observer for mono-variable linear switching systems based on the numerical computation of derivatives of inputs and outputs. Bejarano and Fridman [18] designed a mode observer by a set of Luenberger observers along with a super-twisting based differentiator, which allows the finite time convergence of the observer. Balluchi et al. [15] proposed a mode observer based on a residual generator which is composed of a set of Luenberger observers and works similar to fault detection systems. The observer works based on the available continuous inputs and outputs in the presence of reset states and disturbances. Djemai et al. [19] introduced a mode observer for autonomous switching systems with jumps that can be transformed into the normal form. The observer uses super-twister algorithm to estimate both continuous and discrete states corresponding to the active dynamic. However, the method requires the knowledge of the bound of the state velocity.

In the present study, a mode observer is proposed for transition detection and mode identification of autonomous hybrid systems based on noise-corrupted measurements. The proposed observer is then applied for mode detection of a PSA process. Regarding the known mode sequence and the cyclic nature of the DES model of PSA processes, the mode observer is designed similar to a fault detection system that works based on the comparison of the residuals of two tandem modes of the PSA cycle; one mode is the active mode, and the other is its next mode. As the residual of the active mode increased and the residual of the next mode reduces simultaneously, the mode observer notifies and the next mode becomes the active mode.

The rest of the paper is organized as follows. In Section PSA Process, a first-principle based model of PSA process and its ROM version are explained. In Section Hybrid observer design, observability of the modes and continuous states of the process are analyzed and the proposed hybrid observer is introduced. The hybrid observer is used for complete state estimation of a PSA process for Hydrogen (H_2) purification from a H_2-CH_4 gas mixture and results are illustrated and discussed in Section Results and Discussion. The paper is concluded through the discussion presented in Section Conclusions.

PSA Process

PSA processes are autonomous distributed parameter hybrid systems. As a case study, consider the two-bed, six-step PSA system, illustrated in Fig. 1 along with the corresponding scheduling table for arrangement of the solenoid valves in the switching modes of the process. The adsorption beds contain activated carbon as adsorbent used for separation of a H_2-CH_4 gas mixture. The objective of the process is to obtain a high purity H_2 product from a H_2-CH_4 gas mixture whose H_2 purity is 70%. The structure of the PSA system and the sequence of the operating steps are assumed to be fixed. Each cycle of the mentioned PSA process consists of six sequential steps including Adsorption (ADS), Depressurizing Equalization (DPE), Blowdown (BDN), Purge with product (PRG), Pressurizing Equalization (PEQ), and Re-pressurization (REP).

Nonlinear non-isothermal model for adsorption beds

Mathematical modeling of adsorption processes is well studied in the literature [3,24–27]. The mathematical model of adsorption beds can be obtained based on the total and component mass balances in gaseous and solid phases, along with the energy balance, adsorption isotherm and pressure drop equations. The mechanistic model of the PSA process is described in details in the previous works by the authors [13,27]. It should be noted