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Optimal design and control of pressure swing adsorption process for N_2/CH_4 separation

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ABSTRACT

Pressure swing adsorption (PSA) is a very versatile, albeit complex gas separation and purification technology. Due to its complexity and periodic operation, calculation of the optimal PSA system that simultaneously obtains process design and control decision variables is a complicated task. This work presents detailed design and control optimization study of a two-bed, six-step PSA system aimed at heavy component CH_4 upgrading. The key optimization objective is to enhance product CH_4 recovery while achieving a closed loop product CH_4 purity of 75% for separating 68%N_2/32%CH_4 feed under external disturbances. Traditional sequential and simultaneously design and control approach are employed and compared based on this purpose. The benefits of simultaneous methodology over conventional sequential approach are successfully demonstrated by closed-loop performance results and simulation profiles. The simultaneously design and control methodology has succeeded in synthesizing the optimal PSA cycle which can generate CH_4 recovery as high as 97.30%.

1. Introduction

Coal bed methane (CBM) is a kind of gas mixture that discharged in series of underground coal mining activities. Inside of this mixture, CH_4 is a kind of major component with certain added economic value. CBM usually contains 20–35% of CH_4 as well as other contaminants like N_2, O_2, CO_2, H_2O (Bhadra and Farooq, 2011) Such specific gas constitution made it hard to be utilized directly. Emitting it to atmosphere directly would not only be a waste of clean energy but also lead to severe environmental destruction because the greenhouse warming potential of CH_4 is 25times higher than CO_2 (Krzysztof, 2008; Flores, 1998; Wu et al., 2015; Rosaria et al., 2017). Although low concentration of CH_4 cannot be utilized, secondary-quality methane (30–95%) can be used for electricity generation or fuels (USA EPA, 2005). Thus, recovering CH_4 from CBM is a kind of activity that could converts waste into wealth and capture greenhouse gas to avoid potential global warming (Karapidakis et al., 2010; Börjesson and Berglund, 2007).

To separate and enrich CH_4 from CBM, many chemical engineering processes like cryogenic distillation, membrane and pressure swing adsorption (PSA) or vacuum pressure swing adsorption (VPSA) have already proved to be feasible (Zhong and Daraboina, 2013; Huang and Paul, 2007; Cavenati et al., 2006). Although cryogenic distillation is nearly suitable for all kinds of separation process, its enormous energy consumption could be the biggest drawback considering the specific CBM constitution and physical properties. For method of membrane separation, it is difficult to make a proper trade-off between an ideal selectivity and lower industrial-scale construction cost considering the present technical state. PSA is much more suitable for this gas mixture comparing with the former two methods because of its low cost in energy consumption and highly automatic operation (Liu et al., 2011).

Since its first practical application in later 1950s, PSA and VPSA have been used in many mixtures separation and there is no exception in CBM separation and concentration (Hiro et al., 2005). Gomes and his coworkers simulated the VPSA process to recover CH_4 from coal-seam methane then verified their validation by experiments. Results show that CH_4 could be concentrated from 50% to no less than 90% with recovery of 60% by 2-bed 4-step operations (Gomes and Hassan, 2001). Besides, Olajossy uses both simulation and experimentation to study processes of CH_4 recovering from CBM. Their pilot plant research was carried out based on their

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simulation prediction and reached a recovery of no less than 96% (Olajossy et al., 2003).

From above work, it can be easily known that researchers have used both simulation and experiment to study the PSA system. However, as a result of the fact that the performance of a PSA process correlates, it is difficult to get the optimal condition and control it under outside disturbances just by experiments and pilot plants. Luckily, in the last three decades, the systematical mathematical models of PSA system have been established and simulated successfully. Based on this, it is now often used the sequential-based approach to get the best simulation results while control the system under external disturbances. This means the model-based system would be optimized to achieve certain goals while meet some constraints firstly. Then, the optimized condition is simulated within some unknown scenarios and use controllers to make it satisfied some production standards (Sircar, 2006; Jayaraman et al., 2004; Khajuria and Pistikopoulos, 2013).

For the optimization part, Smith and Westerberg presented a mixed-integer non-linear programming (MINLP) to optimize the operation cost (Smith and Westerberg, 1992). Then Nilchan proposed a simultaneous discretization in both spatial and temporal and converts the partial differential algebraic equations (PADEs) into nonlinear algebraic equations and made it possible to use the NLP solver to solve it (Nilchan and Pantelides, 1998). Soon afterwards, Ko et al. configured the r-SQP to decide the optimal operate variables like feed flowrates, step pressure and time duration (Ko and Moon, 2002). Huang et al. built a rigorous PSA model and solved it in software gPROMs. Also in Sun's work, she built a fundamental PID control strategy and testified it with several kind of external disturbance (Huang et al., 2008; Sun et al., 2015).

Then in the control part, a controller is needed for the chemical system. A few numbers of studies have focused on control system in chemical unit operation like distillation and crystallization. For example, Singh et al. designed a proportional-integral-derivate (PID) controller and compared its performance with open loop simulations (Singh et al., 2014). Torre et al. established a model predictive controller for periodic adsorption process (Torre et al., 2005). Khajuria et al. proposed a model predictive control (MPC) strategy for a H_2/CH_4 PSA separation system and tested the performance of the MPC controller and compared it with the PID controller (Khajuria and Pistikopoulos, 2011).

In industrial PSA separation processes, there are inevitable unknown disturbances that may induce performance variables changes. This means that the desired quality of product needs to be controlled and enhanced through incorporating proper controller during the design stage. In traditional sequential approach, optimization is carried out firstly to get the best operate condition. External disturbances are then added into the newly got optimal condition and applied certain control strategy to make product meet necessary constraints. Such working order may possibly meet product's quality demand but loses its best operation condition after the second step. Thus, developing a systematic integrated design and control strategy that satisfied the design target during both steady state and transient in the presences of various unknown disturbances and process has become urgent to PSA systems (Sakizlis et al., 2004). Simultaneous design and control PSA system employing the optimization-based approach has significant meaning for its practical operation in industries. Focusing on this point, we have built a dynamic optimization approach and used it in the PSA system.

This paper presented a systematic model-based simulation, optimization and control of the PSA process for methane production. A PDAEs-based model of the vacuum pressure swing adsorption process for separation of CH_4 from CBM mixture is studied with feed composition of $68\%N_2/32\%CH_4$. The accuracy of mathematical models was verified by a series of experiments that differ in feed and replacement feed flowrates from 32 m^3/h to 50 m^3/h. Based on the cyclic steady state that reached from the simulation work, the sequential approach that optimizing recovery of CH_4 to maximum on the basis of product purity not less than 75% with certain design constraints (pressures, valve constant, replacement gas flowrate and evacuation gas flowrate) was firstly carried out. Using the optimization results, disturbance like transient impulse in feed flow rate was added into the system while employing the embedded PID controller to manipulate the adsorption step time duration to maintain product purity as no less than 75%. Afterwards, the newly built simultaneous optimization and control framework was presented and added the same external disturbance onto it with same optimization objective and constraints. Finally, we compared the simultaneous optimization-based simulation performances with sequential-based approach. Results show that comparing with traditional sequential approach, the simultaneous approach has shorter response time, better inside operation condition and prior performance facing external disturbances.

2. PSA model validation

2.1. PSA model

A systematical PSA model should be able to describe the inherent dynamic changes of the process as time goes on while other constraints like definition of cycle steady state and boundary conditions within it. In this paper, such a PSA model as well as its optimization and control framework is built in gPROMS.

The following assumptions are used for the PSA bed model:

(1) The gas phase behaves as an ideal gas.
(2) No radial variation in gas concentration, temperature and pressure.
(3) Pressure drop along the bed is calculated by the Ergun equation.
(4) Thermal equilibrium between the gas and solid phases.
(5) The porosity of bed and adsorbent particle is uniform along the bed.
(6) Adsorption rate is approximated by linear driving force (LDF) approximation model with a single lumped mass transfer coefficient.
(7) Adsorption behaviors are described by Langmuir isotherm model.

In this work, the competitive adsorption behavior is described by the extended Langmuir isotherm based on pure component data that presented in Eq. (5). Activated carbon (AC) is selected as the adsorbent in this paper just as most N_2/CH_4 research did. The kinetic adsorption rate is represented by the linear driving force (LDF) approximation model, which is described in Eq. (6). Other mathematical equations and sub-models like valves could be seen in Tables 1–3 list key parameters for N_2/CH_4 system. Corresponding boundary conditions for individual steps are listed in Tables 4 and 5. As most papers did, we also used purity and recovery to assess the performance of a PSA process and the definition of these two parameters are listed in Table 6.

2.2. Cycle scheme design

In general, a PSA system usually contains two or more adsorption beds interacting with each other via a net of solenoid valves. Different steps are achieved by a system that controls opening of different valves in different steps. The cycle scheme for a heavy