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Detailed simulation of dual-reflux pressure swing adsorption process

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HIGHLIGHTS

- Aspen Adsim® model for simulating realistic DR-PSA process scenarios is presented.
- The model is validated against 19 experimental DR-PSA runs.
- Model predictions are in good agreement with experimental results.
- Effect of feed position on process performance is also assessed via simulations.

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ABSTRACT

A model for the detailed simulation of dual-reflux pressure swing adsorption process developed in the frame of the commercial software Aspen Adsim® is presented. For validation purposes, simulations were performed and model predictions were compared with published experimental results. At cyclic steady-state, model predictions were found to be in good agreement with reported experimental results in terms of (i) average ethane mole fraction in heavy product, (ii) average nitrogen mole fraction in light product, (iii) instantaneous heavy product composition profiles, and (iv) instantaneous column composition profiles. The predicted and experimental trends obtained by analyzing the effect of various operating parameters (light reflux flowrate, duration of feed/purge step, heavy product flowrate and mole fraction of heavy component in binary feed gas mixture) on process performance are also comparable. Overall, this simulation technique of dual-reflux pressure swing adsorption can serve as an effective tool for process design, cost reduction of laboratory and/or plant trails, and enhanced process understanding.

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1. Introduction

Since its inception more than half a century ago, the technology of pressure swing adsorption (PSA) has been widely studied and applied, becoming today the method of choice for the separation and/or purification of many gaseous mixtures. Some of its most popular industrial applications include hydrocarbon separation, hydrogen purification, air drying, and air separation. PSA systems employed for the processing of binary feed gas mixtures can be categorized into three main types: (i) stripping, (ii) rectifying and (iii) dual-reflux.

Stripping PSA systems are based on the Skarstrom cycle (Skarstrom, 1959) and are capable of producing only the light product (weakly adsorbed; in the following referred to as species *B*) at high purity, since the purity of the heavy product (strongly adsorbed; species *A*) is confined by thermodynamic constraints (Subramanian and Ritter, 1997). Rectifying PSA systems, developed by Diagne et al. (1994) and Ebner and Ritter (2002) and also known as enriching reflux PSA (Yoshida et al., 2003), have thermodynamic constraints on the purity of the light product, thus resulting in the capability of producing only the heavy product at high purities. In contrast, the purity of both the products is thermodynamically unconstrained in dual-reflux pressure swing adsorption (DR-PSA; Leavitt, 1992): consequently, DR-PSA processes are capable of achieving complete separation of binary feed gas mixture, thus producing two pure-component streams.

A typical DR-PSA unit comprises of a combined two-bed system with feed injection in a given position along the axis of the adsorption column. Such position (Z_F) divides each bed into two sections: '*Stripping Section*' (*SS*) and the '*Rectifying Section*' (*RS*). Two reflux streams (so the name DR-PSA), light reflux (*LR*, pure *B*), and heavy reflux (*HR*, pure *A*), are respectively injected at the *SS* and *RS* end of each column during constant pressure steps. Depending on the column operating pressure (high pressure, P_H, or low pressure, P_L)

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to which the binary feed gas mixture is supplied and the type of gas (A or B) with which the pressure swing is carried out, four different cycle configurations can be identified (Kearns and Webley, 2006):

(i) DR-PL-A: feed to P_L and pressure swing with A;
(ii) DR-PL-B: feed to P_L and pressure swing with B;
(iii) DR-PH-A: feed to P_H and pressure swing with A;
(iv) DR-PH-B: feed to P_H and pressure swing with B.

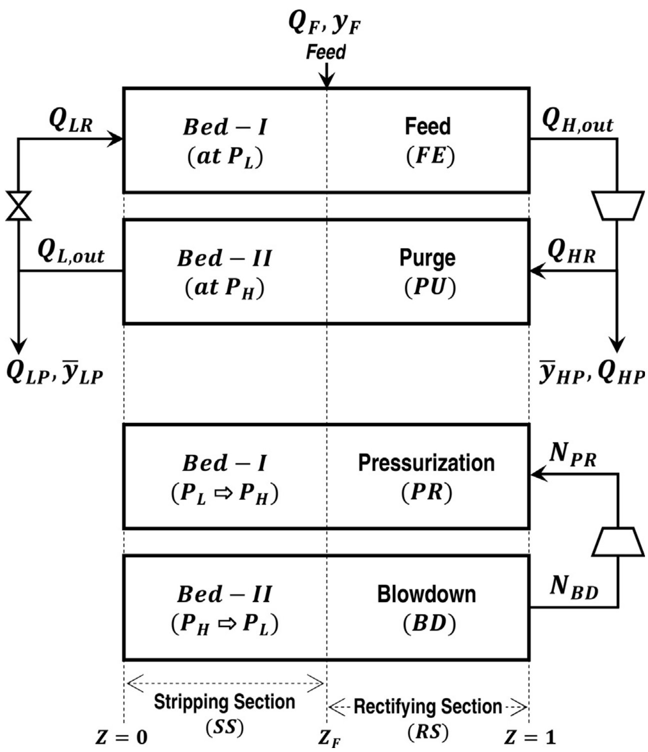

Fig. 1. DR-PL-A cycle steps and flows.

Gas separation processes based on DR-PSA have been studied experimentally in the literature. Diagne et al. (1994, 1995a, 1995b) explored the application of this process to the CO_2 removal from air using zeolite 13X as adsorbent. In these studies they demonstrated that feed gas containing 20% CO_2 can be concentrated to values higher than 94% in the heavy product stream by proper selection of the operating conditions. More recently, McIntyre et al. (2010) conducted experiments using wood-based activated carbons in DR-PL-A configuration for the recovery and enrichment of dilute ethane from nitrogen. In this extensive study, they performed 19 runs for 1500–3000 cycles each and analyzed the effect of various operating parameters on process performance: light reflux flowrate, duration of feed/purge step, heavy product flowrate and feed mole fraction of the heavy component. It was demonstrated that the average of these 19 runs with an ethane feed concentration of 1.38 vol% gave an ethane enrichment of 45.8 times (63.2 vol%) and ethane recovery of 84%, while producing N_2 at high purity (99.8 vol%) and recovery (> 99%). These experimental studies proved that both the light and heavy products can be obtained at high purities using DR-PSA systems.

Various modeling tools ranging from very simple to complex have been reported in the literature for the design and optimization of PSA units (cf. Ruthven et al., 1994; Spoorthi et al., 2011; Thakur et al., 2011; Sivakumar and Rao, 2011a, 2011b, 2012). The simplest modeling approach (usually indicated as equilibrium theory) involves a large set of simplifying assumptions, such as instantaneous linear equilibrium throughout the column, isothermal conditions, negligible mass transport resistances and axial mixing, negligible pressure drop, and ideal gas behavior. The resulting equations have been solved by the method of characteristics (Rhee et al., 1986) and its solution for conventional PSA systems was fully detailed by Knaebel and Hill (1985). Equilibrium theory was applied to DR-PSA systems by Ebner and Ritter (2004),

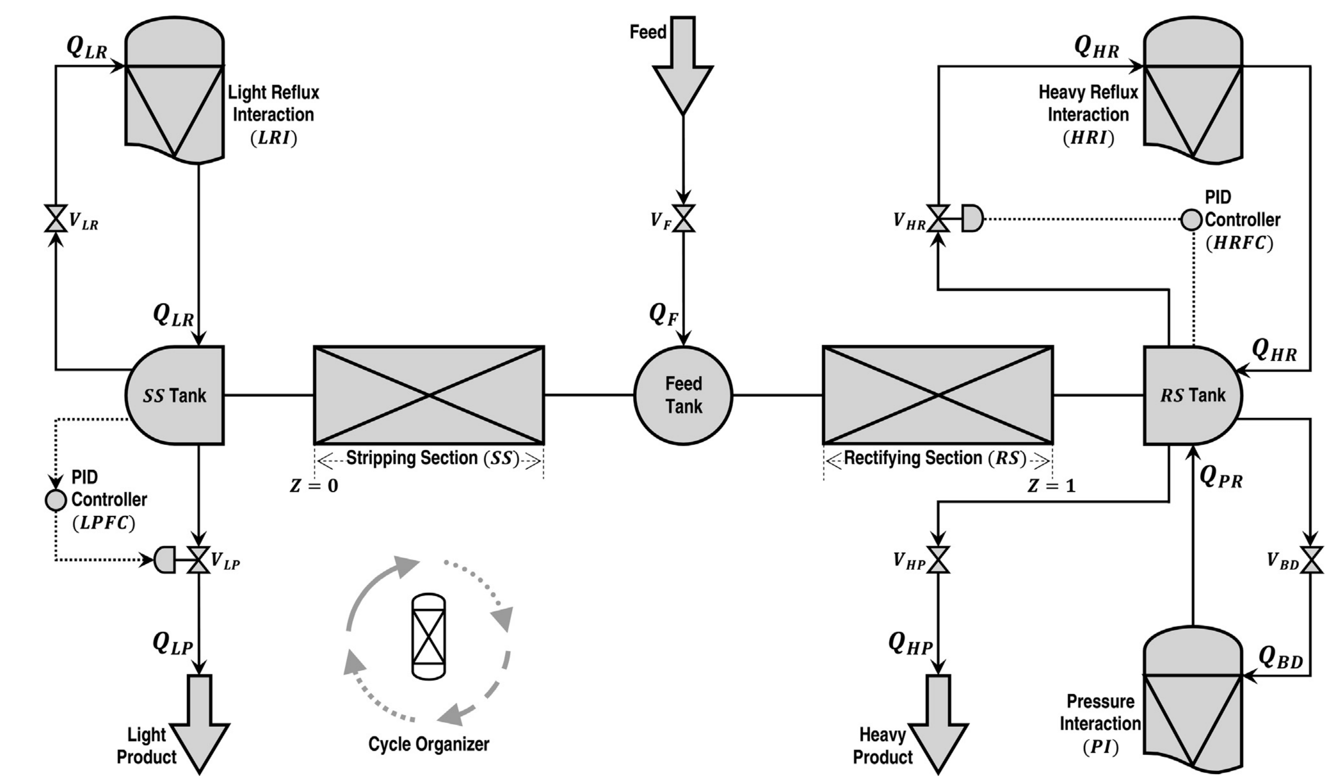

Fig. 2. Schematic representation of DR-PL-A process simulation flowsheet.

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