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Modelling and evaluation of dual reflux pressure swing adsorption cycles: Part II. Productivity and energy consumption

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Abstract

In this second part of our dual reflux PSA study, we have examined the power and productivity tradeoffs of all of the dual reflux cycles developed in Part I. It was found that the concentration of heavy component in the feed is the primary variable that influences the choice of dual-reflux configuration. Feed to the high-pressure bed and equalisation, pressurisation and blowdown with the strongly adsorbed component is favoured at low concentrations of heavy component in the feed gas. Feed to the low-pressure bed and equalisation, pressurisation and blowdown with weakly adsorbed component is favoured for high concentrations of heavy component in the feed gas. For highly selective adsorbents, the differences between the work-productivity tradeoff curves for the four configurations are quite distinct, becoming less distinct as the ease of separation decreases.

Keywords: Pressure swing adsorption; Dual-reflex; Gas seperation; Cyclic adsorption process; PSA design

1. Introduction

Optimisation of PSA systems is an active area of research with many studies contributing to this important field. For example, Cruz et al. (2003, 2005) have recently addressed this issue. Most of the studies to date have dealt with the optimisation of a PSA process once the cycle has been specified i.e. determine the optimal operating and adsorbent parameters to yield highest throughput, recovery, purity etc. There have been virtually no studies which allow the user to select a suitable cycle given only the properties of the adsorbent and the feed concentration. In this study, we examine this aspect of PSA optimisation for a subset of possible cycles: the dual-reflux cycles.

The configuration of the four dual reflux options developed in Part I have widely varying power requirements and productivities. What is the practising engineer to make of these options? What we seek in this part of our study is a set of guidelines to assist initial selection of the appropriate cycle in order to accomplish a specified separation given a particular adsorbent and feed composition. We go about this goal by calculating the work required and productivity for each of the four options for a range of feed compositions, and adsorbent type and comparing the options, seeking clear trends which will help the user select a cycle for investigation.

2. Energy consumption and productivity

The energy (work) consumption of all DR-PSA configurations developed in Part I is determined by the pressure ratio and quantities of gas flowing through the compressors in each step. Compressors are assumed to be isentropic (adiabatic) single-stage (100% efficiency) with an aftercooler to reduce the discharge gas temperature back to the PSA operating temperature. The comparative nature of this study means that the specific compressor/aftercooler arrangement selected is not vitally important because the same assumptions will apply to all four configurations. The number of compressor stages may vary for real PSA plants, but there is always at least one compressor stage for small scale PSA plants. Although a real-world multiple stage compressor with intercooling would reduce the power

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consumption, such a unit would also have an efficiency of significantly less than 100% which would offset this work usage reduction. Therefore, this simple arrangement will be a reasonable approximation of more complex compressor/aftercooler arrangements. The specific work (per kmol) of the compressor is given by the adiabatic compression equation, where 1 and 2 denote the inlet and outlet conditions:

$$\hat{W}_{comp,in} = \frac{\gamma R T_1}{\gamma - 1}\left[\left(\frac{P_2}{P_1}\right)^{(\gamma-1/\gamma)} - 1\right]. \tag{1}$$

During the FE/PU step, gas is compressed from P_L to P_H at the constant flowrate $\dot{N}_{H,in}$ for time t_F. The compressor work during the FE/PU step is (for all four configurations):

$$W_{comp,FE/PU} = \dot{N}_{H,in} t_F \frac{\gamma R T_{env}}{\gamma - 1}\left(\left(\frac{P_H}{P_L}\right)^{(\gamma-1)/\gamma} - 1\right). \tag{2}$$

During the PR/BD step, the compressor discharge pressure varies from P_{int} to P_H, while the suction pressure varies from P_{int} to P_L, where P_{int} is the intermediate pressure obtained at the end of the equalisation. Integrating (2) with moles of gas for the cycles compressing A gas during these steps (see part I, configurations DR-PL-A and DR-PH-A):

$$W_{comp,PR/BD} = \frac{\gamma \varepsilon A_{CS}}{(\gamma - 1)\beta_A}\int_{P_{int}}^{PH} \times\left(\left(\frac{P_2}{P_L + P_H - P_2}\right)^{(\gamma-1)/\gamma} - 1\right) \mathrm{d}P_2. \tag{3}$$

For the cycles compressing B gas during the PR/BD steps (DR-PL-B and DR-PH-B):

$$W_{comp,PR/BD} = \frac{\gamma \varepsilon A_{CS}}{(\gamma - 1)\beta_B}\int_{P_{int}}^{PH} \times\left(\left(\frac{P_2}{P_L + P_H - P_2}\right)^{(\gamma-1)/\gamma} - 1\right) \mathrm{d}P_2. \tag{4}$$

Eqs. (3) and (4) are evaluated numerically in this study.

Productivity of the adsorbent is usually defined as the number of moles of product produced per unit quantity of adsorbent per unit time. Cycle time therefore directly impacts productivity—faster cycles lead to greater productivity (provided recovery remains constant). In equilibrium-based models such as those employed here, the actual cycle time used is irrelevant (although step times appear in the equations they are "intermediate" variables useful for conducting the calculations). For example, the flow rates can be varied without changing the quantities of gas entering/leaving the beds during each step—an increase in flowrate merely decreases the step duration and vice-versa. What is important is the number of moles entering or leaving the beds on a per cycle basis. It is assumed that all configurations may be operated faster or slower as desired. Therefore, a more useful measure of productivity for equilibrium models is moles of product produced per unit mass of adsorbent *per cycle*. Furthermore, dual-reflux PSA is unique in that the recovery of both products is 100%, hence the productivity (on a per cycle basis) is directly related to the feed throughput or moles of feed per unit mass adsorbent per cycle (with the feed mole fraction being the constant of proportionality). We are therefore entitled to use kmol of feed gas processed per cycle per unit mass of adsorbent as a surrogate for productivity. We have chosen this because the calculations are greatly facilitated by being able to specify a feed rate (kmol/s) and then calculating the required feed time which in turn gives the number of moles fed to the bed.

3. Results and discussion

This study focuses on the relative performance of the four DR-PSA configurations. Many operating parameters do not cause much (if any) change in relative system performance and thus were held constant. These include bed length (1 m), bed cross-sectional area (1 m^2), and feed flowrate (0.001 kmol/s). As discussed above, although the feed flow *rate* is fixed, the moles of feed to the beds are not—the required feed time is calculated for each case. The fixed adsorbent physical properties are taken from the Linde 5A $\frac{1}{16}$ adsorbent typically used for air separation (N_2 is strongly adsorbed, O_2 weakly adsorbed) (source: Linde). The adsorbent voidage is 0.37, bulk density 800 kg/m^3 (yielding solid density of 1270 kg/m^3) and isotherm parameter of weakly adsorbed gas is k_{B0} of $4.748058749 \times 10^{-10}$ kmol/kg kPa. Low-pressure P_L is fixed at one standard atmosphere (101.325 kPa), and operating temperature fixed at 25 °C (298.15 K). Feed gas is assumed to be available at the required feed bed pressure (either P_L or P_H).

The variables are feed composition y_F, pressure ratio P_H/P_L (set by varying P_H) and separation factor β (by varying isotherm parameter k_{A0}). Feed composition y_F and separation factor β each take the potential values of 0.10, 0.50 and 0.90 to cover low, medium and high values of the available feed gas compositions and adsorbent selectivities. Pressure P_H was allowed to vary from 102–1000 kPa continuously initially and later in increments of 50 kPa.

Table 1 shows the values of P_H for which CSS was reached for various values of β, y_F and cycle configuration.

The empty cells in Table 1 indicate that the cycle did not converge for any P_H tested. This was invariably because the stripping shock wave did not fully develop. The rectifying shock *always* develops under all conditions, as it does in a pure rectifying cycle (Ebner and Ritter, 2002). It was also found that the z_F values become closer to the pure B end of the bed as the pressure ratios increased, resulting in a process that approaches a rectifying cycle. It was decided that all cycles where z_F is less than 5% of the bed length from the pure B end of the bed would be impractical. The cycles in Table 1 where the upper P_H limit is less than 1000 kPa had the upper limit set by this z_F restriction, not by the stripping shock development restriction.

The reflux rates in all cases can be stated as the ratio of pure B reflux to feed rate, $\dot{N}_{L,in}/\dot{N}_F$. It was found that for all four configurations, the reflux rate increases with β and decreases as y_F and P_H/P_L increase. Fig. 1 demonstrates the reflux