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Visualization of multi-objective decisions for the optimal design of a pressure swing adsorption system

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ABSTRACT

Optimization based process design tools are most useful when combined with the human engineer's insight. Further insight can be gained through the use of these tools by encouraging the exploration of the design space. Visualization is one technique which makes it easier for an engineer to understand the designs identified by an optimization tool. There are many visualization techniques but most are for individual process designs or for understanding the behavior a design space when a single design objective is considered. Most design problems, however, are multi-objective. This paper presents a multi-objective visualization method and applies it to the industrially relevant design of pressure swing adsorption systems.

1. Introduction

Computer based industrial process design is a challenging task due to a combination of factors, with complex mathematical models and multiple often conflicting objectives being just two of these factors. Multi-objective optimization tools provide a mechanism by which designs can be identified and trade-off curves generated. These allow the engineer to gain insight into the key characteristics of potentially good designs before moving on to more detailed simulations and pilot plant tests. Insight is gained by analyzing the designs and the trade-off curves and one of the most useful techniques for analysis is visualization. This paper demonstrates the potential of multi-dimensional visualization for a case study of industrial relevance.

2. Mathematical model

Pressure swing adsorption (PSA) is a cyclic adsorption process for gas separation and purification. PSA systems have the potential of achieving a higher productivity for CO_2 capture than alternative separation processes [1], such as absorption. However, an efficient and cost-competitive PSA unit is one that achieves high levels of purity and recovery of the product, two competing objectives [2]. Multi-objective optimization methods are therefore required to generate suitable trade-off curves and that allow an engineer to identify those designs which best resolve the conflict in these objectives.

Optimization based design methods require mathematical models of the system. Mathematical models for PSA processes are governed by partial differential algebraic equations (PDAEs). The performance of a PSA process is usually based on its behavior at *cyclic steady state* (CSS). At CSS, the physical conditions at the end of a cycle are identical to those at the beginning of that cycle. To reach CSS from start-up may take hundreds or thousands of cycles [3]. The simulation of a PSA process, therefore, is computationally challenging since the resulting system of PDAEs that needs to be solved is usually large and stiff. Also, hyperbolic PDAEs, which often are used, tend to generate solutions suffering sharp fronts in the gas concentration profile, and non-physical oscillations due to shock waves [4]. Because of this, the task to perform PSA simulation can be very time-consuming; a single simulation to CSS can take minutes, hours, or even days. Most optimization approaches thus either use simplified governing equations or limit their search to a reduced design space [3]. More recently, surrogate modeling techniques have been used to address the computational challenge [5].

Given suitable models and appropriate optimization methods, trade-off curves may be generated. The challenge then becomes one of understanding what characteristics of the designs identified are important for the objectives considered, with the aim of enabling an engineer to choose one or more designs for further, more detailed, analysis. Visualization becomes a key tool in the engineer's repertoire to address this challenge.

To illustrate this challenge and a potential approach, we have chosen a case study from literature that is challenging and sufficiently complex (see [6]) while not intractable computationally. Fig. 1 shows the process steps involved in one PSA design with the process configuration shown

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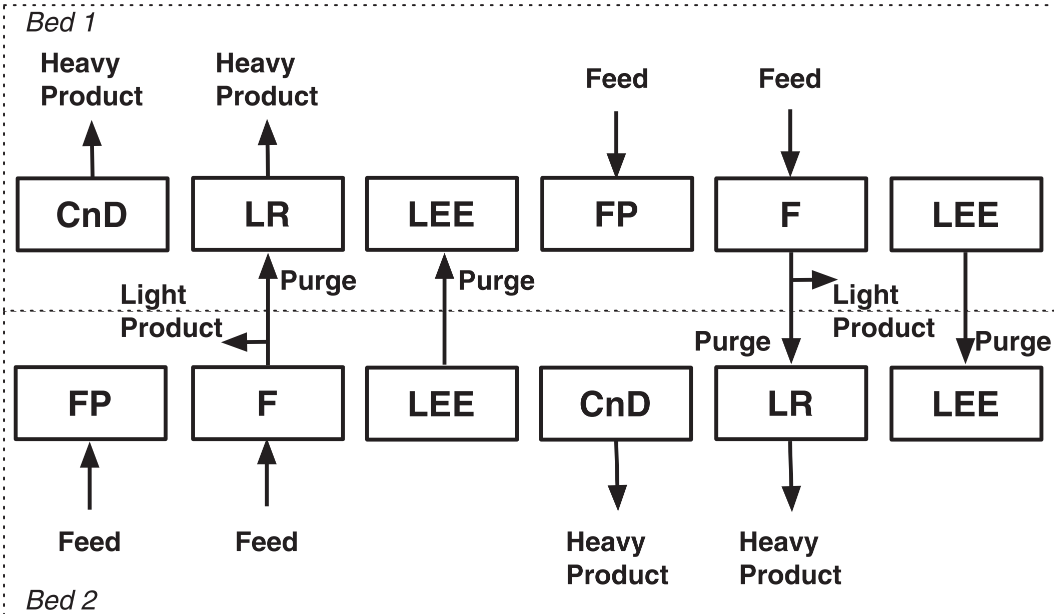

Fig. 1. The processing stages for the 2-bed/6-step PSA Skarstrom cycle process.

in Fig. 2. This is the PSA Skarstrom cycle with an added pressure equalization step as proposed in [6]. The PSA cycle considered is defined by the following 6 steps: feed pressurization (FP), feed/adsorption (F), light end equalization (LEE), countercurrent depressurization (CnD), light reflux (LR), and light end pressurization (LEE). The FP step is characterized by a high-pressure gas mixture entering the bed while not permitting any gas to leave. The F step is characterized by a high-pressure bed with feed entering the bed. LEE is a pressure equalization step and is typically used to conserve the energy of the system. CnD is depressurization with the same flow direction as the adsorption flow. LR is countercurrent low-pressure desorption with light product purge.

The transitions between the process steps are regulated by the stem positions of the valves. The 7 valves involved are shown in the process configuration in Fig. 2. The system is symmetrical with the axis of symmetry going through the feed and vent units. On both sides of each bed is a bed header which is usually used to ensure a homogeneous flow distribution in the bed. The units labeled "Feed", "Vacuum" and "Vent" provide the boundary conditions for the PSA system. Briefly, the Feed unit is an inlet which provides the gas mixture to separate; the Vacuum unit is an outlet which provides vacuum pressure for the purge and blowdown steps; the Vent unit is an outlet at atmospheric pressure. These three units are referred to as feed units. The tanks next to the feed units are buffering the flow so that the pumps can be operated continuously. The tanks and bed headers are connected by valves which control the flow rates in the system and thus the cycle steps. This PSA system is considered for the recovery of CO_2 from the flue gas in a power plant. With the pressure equalization step the CO_2 purity can be enriched [6] at the price of a small increase in power consumption. The use of LR steps typically leads to an improved product recovery. One expects that with higher CO_2 purity, the system will consume more power at the vacuum pump. The system parameters that are considered fixed are given in Table 1.

The adsorption beds are packed with zeolite 13X pellets [7]. The stem positions open and close at specific times during the course of a cycle to control the PSA operation. See Table 2 for the stem positions for the different process steps of this 6-step PSA Skarstrom cycle. Here 0 means that the valve is closed, 0.5 half open, and 1 fully open. The PSA cycle is performed through the coordinated operation of the 7 valves. The feed unit supplies a gas mixture of constant pressure, temperature, and feed composition, and therefore held at the initial operating conditions.

The mathematical equations involved describe conservation of mass and energy, pressure profiles, and adsorption kinetics in an adsorbent bed. There are mass balance equations for the individual gas components and non-isothermal energy balance equations for the adsorbate in the gas phase, the adsorbate in the solid phase, and for the bed wall. The model is an axial dispersed plug flow model, where the axial dispersion term represents the contribution to axial mixing. The pressure drop along the bed is given by the well-known Ergun equation [3] The Ergun equation is the steady-state momentum balance of gas flow and relates the pressure drop to the gas velocity along the adsorbent bed. The mass transfer is modeled using the linear driving force (LDF). The LDF model is a linear approximation of the homogeneous diffusion equation for the mass transfer rate. Moreover, the Langmuir adsorption isotherm is used in this study with the data provided in [8].

The bed header and the tanks are modeled as continuously stirred tanks, and the flow rate in the feed unit is controlled by valve equations:

$$F = r_j c_v c_T \sqrt{\frac{\left|p_0 - p_{L_b}\right|}{\rho_f}}. \quad (1)$$

Here r_j is the stem position, c_v is the valve coefficient, p_0 and p_{L_b} are the pressures at the two inlets, respectively, c_T is the total concentration and ρ_f is the fluid density. The pressure in the tank is given by the ideal gas law. The boundary conditions for the gas phase concentrations and the enthalpy are given by the Danckwerts boundary conditions for flow into the bed and the no diffusive flux for flow out of the bed.

For further details on the mathematical model considered in this work, see [8].

The computational model used relies on a finite volume scheme using 40 volume elements with a Van Leer flux limiter. The simulation time for a single design configuration ranges between 10 min and an hour, depending on the design configuration used. The PSA cycles are simulated in succession until CSS has been reached. A backward differentiation formula (BDF) of 5th order is used for time integration.

3. Statement of the relevant optimization problem

The PSA design problem is to maximize two conflicting objectives, the product purity and recovery, from a feed with composition 15% CO_2–85% N_2. The CO_2 purity and recovery during cycle k is calculated