17th European Symposium on Computer Aided Process Engineering – ESCAPE17
V. Plesu and P.S. Agachi (Editors)

Modelling and simulation of multi-bed pressure swing adsorption processes

Dragan Nikolic,[a] Apostolos Giovanoglou,[b] Michael C. Georgiadis,[b,c] Eustathios S. Kikkinides[a]

[a]*University of Western Macedonia, Department of Engineering and Management of Energy Resources, Sialvera & Bakola Str., 50100 Kozani, Greece, kikki@cperi.certh.gr, dragan@uowm.gr*
[b]*Process Systems Enterprise Ltd, Thermi Business Incubator, 9th Km Thessaloniki-Thermi, 57001 Thessaloniki-Thermi, Greece, a.giovanoglou@psenterprise.com*
[c]*Imperial College London, Centre for Process Systems Engineering, Department of Chemical Engineering, London SW7 2AZ, UK, m.georgiadis@psenterprise.com*

Abstract

This work presents a generic modelling framework for the separation of gas mixtures using multi-bed Pressure Swing Adsorption (PSA) systems. Salient features of the framework include automatic generation of a superstructure network for an arbitrary number of beds, customizable complexity of adsorbent bed models using one or more adsorbent layers, and efficient and user friendly generation of complex operating procedures. The predictive power of the developed framework has been validated against literature and experimental data. Furthermore, the analysis of a hydrogen purification process from steam methane reforming off gas serves for application purposes of the modelling framework.

Keywords

Pressure swing adsorption; gas separations; dynamic modelling

1. Introduction

Pressure swing adsorption is a gas separation process, which has attracted increasing interest because of its low energy requirements as well as low capital investment costs. The detailed modelling and simulation of single bed PSA systems has received considerable attention in the literature but most of the previous studies focus on relatively simple flowsheets with a small number of beds and simple operating procedures. Furthermore, in many cases simple models have been used to describe the process under question. However, industrial practise indicate that complex gas separations under high product quality requirements (e.g. purity and/or recovery), rely on complex PSA flowsheets with several interconnected beds and complicated operating procedures [1-2]. The detailed modelling of such systems, the automatic generation of the process as well as all feasible operating procedures constitute several challenging tasks.

This work presents a generic modelling framework of multi-bed PSA flowsheets using one or more adsorbent layers. The framework provides the basis for the automatic generation of the PSA flowsheet and all feasible operating procedures. Several case studies are used to illustrate the predictive power of the modelling and simulation approach and the importance of having multi-beds for gas separation.

2. Modelling framework

The framework provides the superstructure of an adsorbent bed network (for an arbitrary number of beds), fully interconnected via gas valves. The superstructure is governed by operating procedures, which open/close appropriate valves according to a given sequence. The different physicochemical phenomena occurring in the plant are hierarchically decomposed into a set of low-level models (such as adsorbent bed, gas valve, and feed and products storage tank models). The gPROMS® modelling and optimization environment has been chosen as a development platform.

2.1. Adsorbent bed models

The detailed modelling of PSA processes has to take into account the simultaneous mass, heat and momentum balances, adsorption isotherm, pore-scale transport and thermo-physical properties of the fluids followed by different sets of boundary conditions at each operating step. Complexity of the adsorbent bed model can be customized, that is adapted to the particular use (for example highly detailed modelling versus simplified models for real-time optimization). Complex boundary conditions have been developed making possible existence of all known PSA operating steps. The model includes following features and provides several options:

- Mass transfer at the pore scale is described by four different theories such as local equilibrium, linear driving force, surface diffusion and pore diffusion.
- Three different thermal operating modes (isothermal, nonisothermal and adiabatic conditions).
- Two different momentum balance (pressure drop) expressions (Darcy's law and Ergun's equation).
- Temperature dependent adsorption isotherms employing linear isotherms (Henry's law) or extended Langmuir type.
- Thermo-physical properties are calculated assuming ideal or real gas.
- Detailed calculation of transport properties through appropriate correlations or analytical expressions.
- Boundary conditions for all different operating steps.

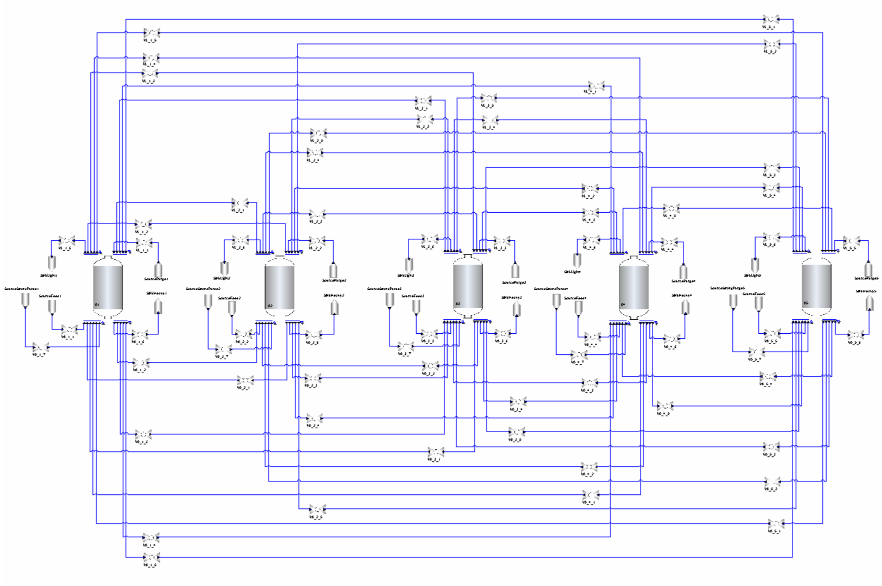

Figure 1. Sample multi-bed PSA flow-sheet with five beds

2.2. The multibed PSA model

The single bed PSA model provides the basis for the automatic generation of the flowsheet via a superstructure of adsorbent bed network. The flowsheet consists of several lower-level models (such as adsorbent beds, gas valves, and storage tanks). A typical five-bed PSA flowsheet is presented in Figure 1. The framework supports an arbitrary number of beds given through an input parameter. All beds are fully interconnected via gas valves and all interactions among beds and flow-rates of all streams are controlled by gas valve equations. The above approach results in the development of a sufficiently general flowsheet that can support all feasible bed interconnectivities and all possible operating steps in every known PSA process.

2.3. Operating procedures/Auxiliary programs

Operating procedures for controlling the execution of multibed PSA processes are highly complex due to the large number of interactions. Hence, an auxiliary program for automatic generation of operating procedures has been developed. This program generates operating procedures for the whole network of beds, according to the given number of beds and sequence of operating steps in one bed. Operating procedures govern the network by opening/closing the appropriate valves at the desired level and changing the state of each bed.

3. Case studies

The adsorbent bed models have been validated against available literature data. The work of Nilchan and Pantelides [3] has been used to validate a single bed linear driving force model, and the work of Shin and Knaebel [4] to validate the single-bed pore diffusion model. In all cases simulation results (not presented here due to space limitations) are in good agreement with the above studies.

The developed framework has been also employed in the separation of H_2 from a $H_2/CH_4/CO/CO_2$ mixture (steam-methane reforming off gas) using activated carbon as an adsorbent. A non-isothermal linear driving force model has been employed. Each PSA cycle involves the following steps: pressurization, adsorption, blowdown, purge and pressure equalization by co-current depressurization and counter-current re-pressurization. Two different configurations have been considered based on the operation of the pressurization step: pressurization by feed and pressurization by the light product (H_2). Several flowsheets including one, four, eight, and twelve beds have been studied under different pressure equalization steps (zero, one, two and three). All configurations have been automatically generated using the auxiliary program. The geometrical data of a column and transport properties have been adopted from the work of Park et al [5]. Three different simulation runs sets have been carried out.

The first simulation run involves configuration 1 (pressurization with feed). The effect of the number of beds and cycle time (due to introduction of pressure equalization steps) on the separation quality has been investigated. The operating procedure involves constant duration of adsorption and purge steps, and constant feed and purge gas flowrates. Simulation results shown in Figure 2a indicate that there is a significant improvement in product recovery (~38%) as the number of beds is increased from one to twelve, while there is a much smaller improvement in product purity (~3%). Moreover, power requirements and adsorbent productivity are decreased (power and productivity of the eight-bed configuration are lower than corresponding of the twelve-bed configuration due to higher cycle time). On the other hand it is noted that the purity of the twelve-bed configuration is slightly lower than the purity of the four and eight-bed. This interesting result can be attributed to the fact that during the third pressure equalization a small breakthrough takes place thus contaminating the pressurized bed.

The second simulation run has been carried out using again configuration 1 (pressurization with feed). In this case, the effect of number of beds for constant power requirements, cycle time and adsorbent productivity on the separation performance has been investigated. The results indicate that there is an over 50% increase in product recovery by increasing the number of beds, from one to twelve, while the resulting improvement in product purity is not as high (~2%). Again, the purity of the twelve-bed configuration is lower than the purity of the eight-bed as analysed in the previous simulation case.

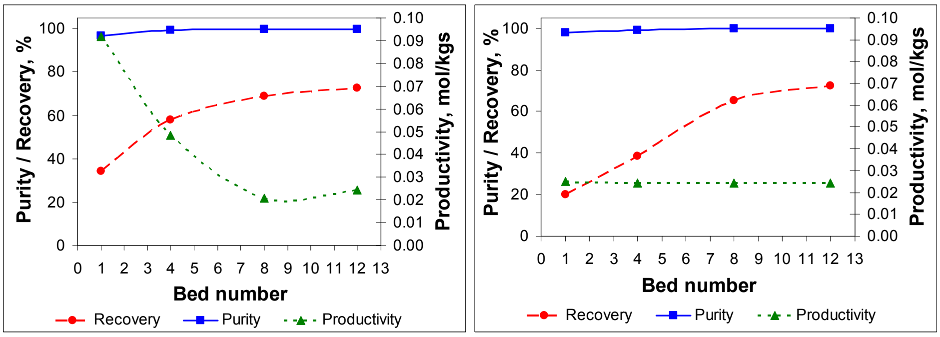

Figure 2. Comparison of results of the first two simulation runs

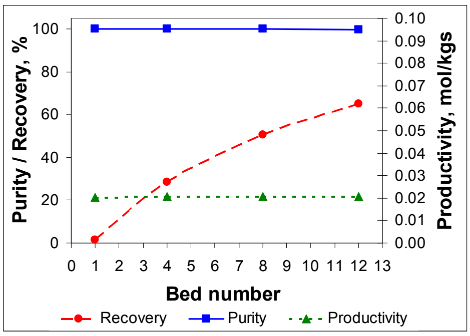

Figure 3. Comparison of results of the third simulation run

The third simulation run has been carried out using configuration 2 (pressurization with light product). The operating procedure involved constant adsorbent productivity, duration of adsorption and purge steps, feed and purge gas flowrates, cycle time, and constant amount of feed processed per cycle. The results shown in Figure 3, demonstrate that the product purity does not change with the number of beds (increase of about 0.1%) but the product recovery is significantly improved (about 64%). Again, the purity of the twelve-bed configuration is lower than the purity of the eight-bed one.

In summary the results illustrate the typical trade-offs between capital and operating costs and separation quality. Thus, increasing the number of beds leads to:

- Higher product purity/recovery
- Higher capital costs (due to larger number of beds)
- Lower energy demands (due to energy conservation because of existence of pressure equalization steps)

4. Conclusions

This study presents a generic modelling framework for the separation of gas mixtures using multi-bed PSA flowsheets. The framework relies on detailed modelling of the process under consideration and automatic derivation of the flowsheet superstructure and operating procedures. Current work focuses on the optimization of multibed PSA systems utilising recent advances in Mixed-Integer Dynamic Optimisation as well as the modelling and optimization of hybrid PSA-membranes.

Acknowledgements

Financial support from PRISM EU RTN (Contract number MRTN-CT-2004-512233) is gratefully acknowledged.

References

1. W.E. Waldron, S. Sircar, Parametric Study of a Pressure Swing Adsorption Process, Adsorption 6 (2000) 179.
2. L. Jiang, L. T. Biegler, V. G. Fox, Simulation and optimal design of multiple-bed pressure swing adsorption systems, AIChE J. 50 (2004) 2904.
3. S. Nilchan, C.C. Pantelides, On the optimisation of periodic adsorption processes, Adsorption 4 (1998) 113.
4. H.S. Shin, K.S. Knaebel, Pressure swing adsorption: An experimental study of diffusion-induced separation, AIChE Journal 34 (1988) 1409.
5. J.H. Park, J.N. Kim, S.H. Cho, R.T. Yang, Adsorber dynamics and optimal design of layered beds for multicomponent gas adsorption, Chem. Eng. Sci. 53 (1998) 3951.