

A ROBUST AND USER FRIENDLY SOFTWARE (TB-PSA-SS) FOR NUMERICAL SIMULATION OF TWO-BED PRESSURE SWING ADSORPTION PROCESSES

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Abstract

The pressure swing adsorption process is a vast operational unit for separation and purification of gaseous mixtures which acts on the basis of ability of solids adsorption features. Nowadays, the PSA process is well-known between numerous processes, and is preferred in contrast to the other routine gas separation methods, particularly for lower capacities, such as cryogenic, and a higher purity. A lot of efforts have been done to develop the processes. In this paper, a new and accurate software (TB-PSA-SS) is presented to simulate the two-bed pressure swing adsorption processes. It is designed in a way that is not limited to the feed type and the system size. It can simulate a two-bed PSA process in experimental and industrial scales for various three-component gaseous systems. The TB-PSA-SS software is produced by MATLAB programming software with the C++ as a basis of its programming language.

Keywords: Simulation Software; Pressure Swing Adsorption; Executable MATLAB Code; Mathematical Solution for Stagewise Process; Forth-Order Ruge-Kutta Scheme; Numerical Simulation.

1. Introduction

Pressure swing adsorption is an important process of gaseous mixture separation. As we know, if its designing principles are not properly considered, we will be faced with a lot of challenges that take some expenses. Proper designing of PSA processes usually is resulted from precise experimental control or pilot plant studies which are used for determination of important designing parameters like bed length, adsorbent type, bed diameters and *etc.* If these studies do not include proper designing principles, they would loss time and money. In other words, unless an accurate and reliable estimation is used for calculation of designing parameters, trial and error method for examination of these factors would be so unusable. A complementary, cheap and reliable method is achieved using a precise mathematical modeling by which adsorption bed dynamic behavior is simulated effectively, so appropriate process design would become attainable. The objectives of mathematical models are:

1. Achievement of primary design and economical evaluation possibility for the usage of PSA processes would become available.
2. To propose experimental purposes and typical industrial studies.
3. To explain experimental results or industrial unit for training purpose.
4. If special model properties are available, they will be used directly for the process design.

However, using of mathematical models cannot be a design tool lonely, because having no access to accurate, general and applicable software for the model is a big challenge. So, up to now different types of programs are presented around the world. We can indicate to AdDesignSTM software as a complete program which is restricted to Michigan University [13]. Here, the presented software (TB-PSA-SS) is a simple practical option which helps the design engineers to be successful in designing of PSA processes desirably, and also provides the ability of designing a suitable pattern, for the desired PSA process at the

least time. It is prepared for Microsoft Windows™ media, and is performed by a graphical user interface (GUI) to make the accessibility easier for the user.

2. Description of Mathematical Model in the Software

For mathematical modeling of adsorption bed, the most significant assumptions are listed below.

1. Ideal gas law for gas phase is considered.
2. Total pressure during adsorption and purge steps, are constant over time.
3. Total pressure during the pressurization, equalization and blow down steps changes with time as a second order equation.
4. Flow pattern is assumed as axially dispersed plug flow model.
5. Equilibrium correlations for gas phase are presented by three-component Langmuir-Freundlich isotherm.
6. The rate of mass transfer is commig from linear driving force (LDF) equations.
7. Radial distribution is negligible.
8. There is a thermal equilibrium between gas and solid phases.
9. Pressure drop along the bed is calculated by Ergun equation.

Model equations for bulk phase in adsorption bed are shown in table 1. In order to solve partial differential equations in each step of the PSA process, common Danckwerts boundary conditions are used [3,4,6,9,15].

Table 1 Model equations [9]

$\frac{\partial C_i}{\partial t} - D_L \frac{\partial^2 C_i}{\partial z^2} + \frac{\partial(C_i \cdot u)}{\partial z} + \rho_p \cdot \left(\frac{1-\varepsilon}{\varepsilon} \right) \cdot \frac{\partial \bar{q}_i}{\partial t} = 0$	(1)
$\frac{\partial C}{\partial t} - D_L \frac{\partial^2 C}{\partial z^2} + \frac{\partial(C \cdot u)}{\partial z} + \rho_p \cdot \left(\frac{1-\varepsilon}{\varepsilon} \right) \cdot \sum_{i=1}^N \frac{\partial \bar{q}_i}{\partial t} = 0$	(2)
$-K_l \frac{\partial^2 T}{\partial z^2} + \varepsilon \cdot \rho_g \cdot c_{p,g} \cdot \left(u \frac{\partial T}{\partial z} + T \frac{\partial u}{\partial z} \right) + \left(\varepsilon_t \cdot \rho_g \cdot c_{p,g} + \rho_B \cdot c_{p,s} \right) \cdot \frac{\partial T}{\partial t} - \rho_B \cdot \sum_{i=1}^N \left(\frac{\partial \bar{q}_i}{\partial t} \cdot (-\Delta \bar{H}_i) \right) + \frac{2h_i}{R_{B,i}} (T - T_w) = 0$	(3)
$\rho_w \cdot c_{p,w} \cdot A_w \frac{\partial T_w}{\partial t} = 2\pi R_{B,i} h_i (T - T_w) - 2\pi R_{B,o} h_o (T_w - T_{atm}); A_w = \pi (R_{B,o}^2 - R_{B,i}^2)$	(4)
$P(t) = a \cdot t^2 + b \cdot t + c$	(5)
$-\frac{dP}{dz} = a \cdot \mu \cdot u + b \cdot \rho \cdot u \cdot u ; a = \frac{150}{4R_p^2} \cdot \frac{(1-\varepsilon)^2}{\varepsilon^2}; b = 1.75 \frac{(1-\varepsilon)}{2R_p \varepsilon}$	(6)
$q_i = \frac{q_{m,i} \cdot B_i \cdot P_i^{n_i}}{1 + \sum_{j=1}^s B_j \cdot P_j^{n_j}}; q_{m,i} = k_1 + k_2 T; B_i = k_3 \cdot \exp\left(\frac{k_4}{T}\right); n = k_5 + \frac{k_6}{T}$	(7)
$\frac{\partial \bar{q}_i}{\partial t} = \omega_i \cdot (\dot{q}_i - \bar{q}_i); \omega_i = \frac{15D_{ei}}{r_c^2}; \frac{15D_{ei}}{r_c^2} = C_i \cdot P_r^{0.5} \cdot (1 + B_i \cdot P_i)^2$	(8)

3. The Two-Bed Pressure Swing Adsorption Processes Simulator Software (TB-PSA-SS)

When TB-PSA-SS file is run, GUI window will be opened (Fig.1).

After entering required input data in its place, we can wait for the software executing by clicking the Run key. It should be observed that its pattern enables us to estimate the effect of pressure equalization step on PSA process performance. After finishing simulation, software results including component's concentration in gas and solid phases, gas phase and bed wall temperature, total gas phase pressure and gas velocity at different steps will be saved in software directory in a txt format. After that cyclic diagrams of component

concentration in gas phase, gas flow rate and temperature will be displayed online in GUI page which can be selected by user. A typical simulation of TB-PSA-SS is shown in Fig.2.

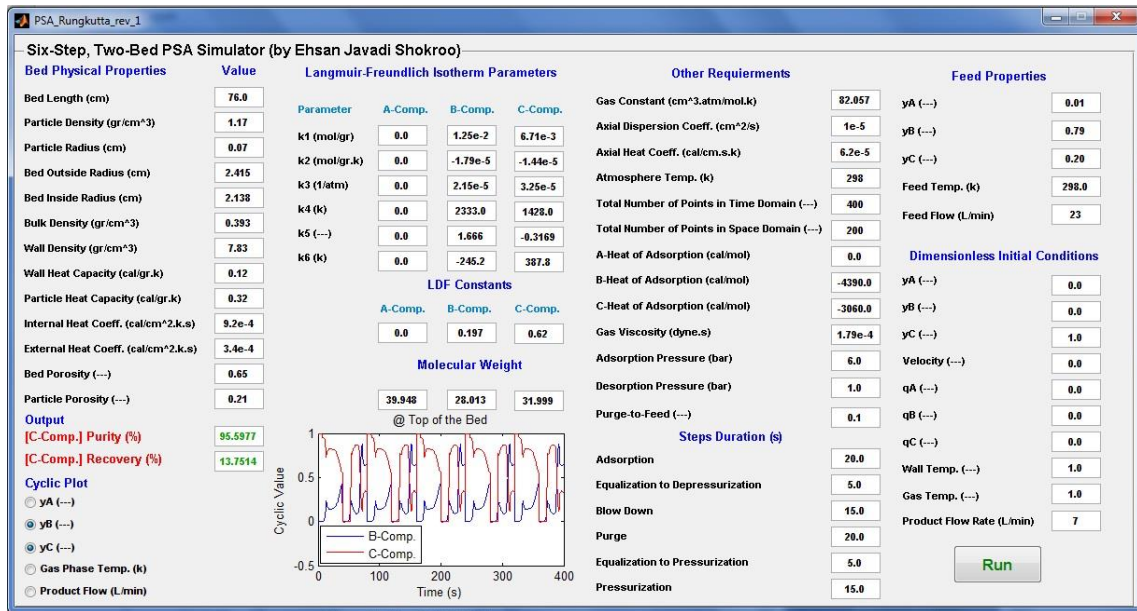


Figure 1 Picture of TB-PSA-SS GUI window.

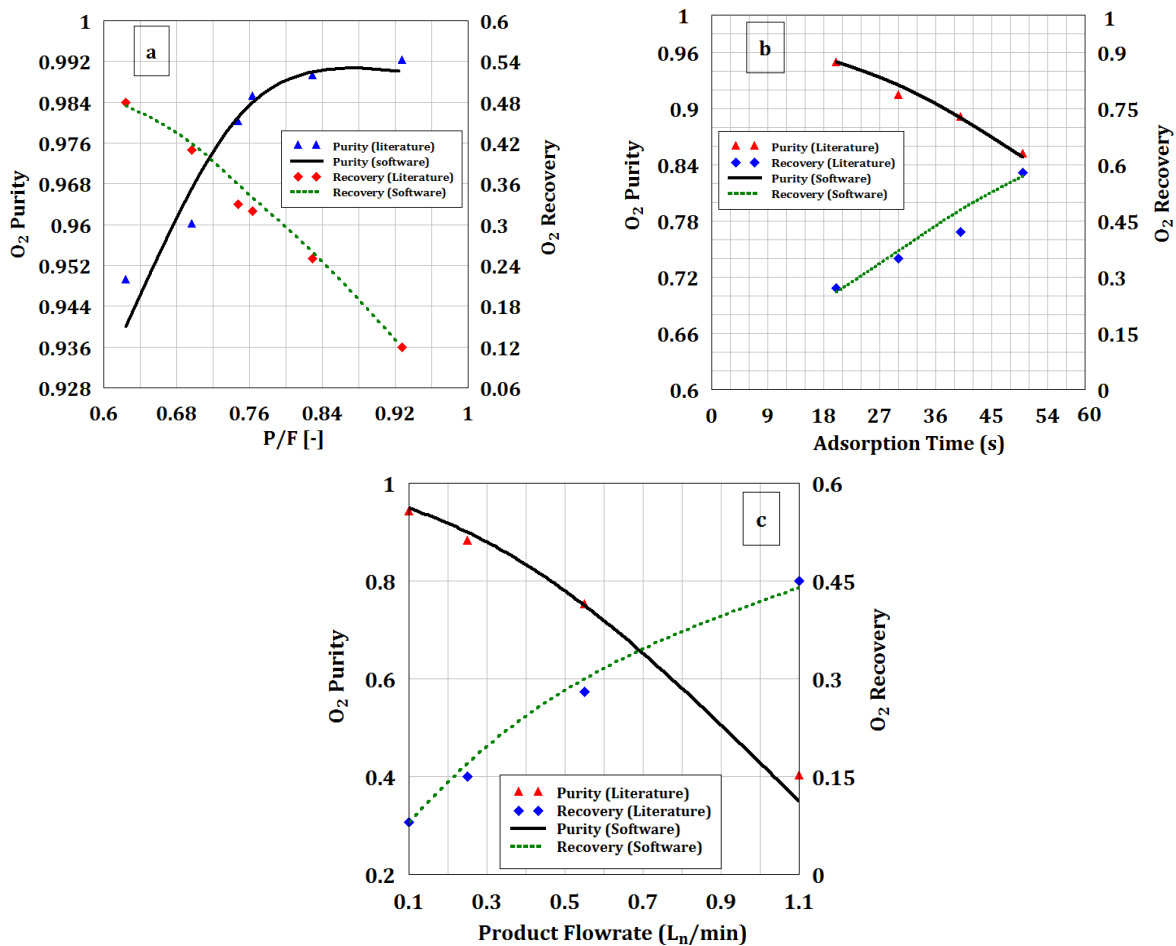


Figure 2 Examples of TB-PSA-SS simulation result for air separation by Zeolite 5A, (a: Jee *et al.* [9]; b: Jee *et al.* [10]; c: Mendes *et al.* [12]).

In accordance with references, curves trends are completely reasonable [9,10,12]. Also online simulation results are shown in Fig. 3. The solution algorithm of each step of the process and cyclic algorithm is shown in Fig. 4.

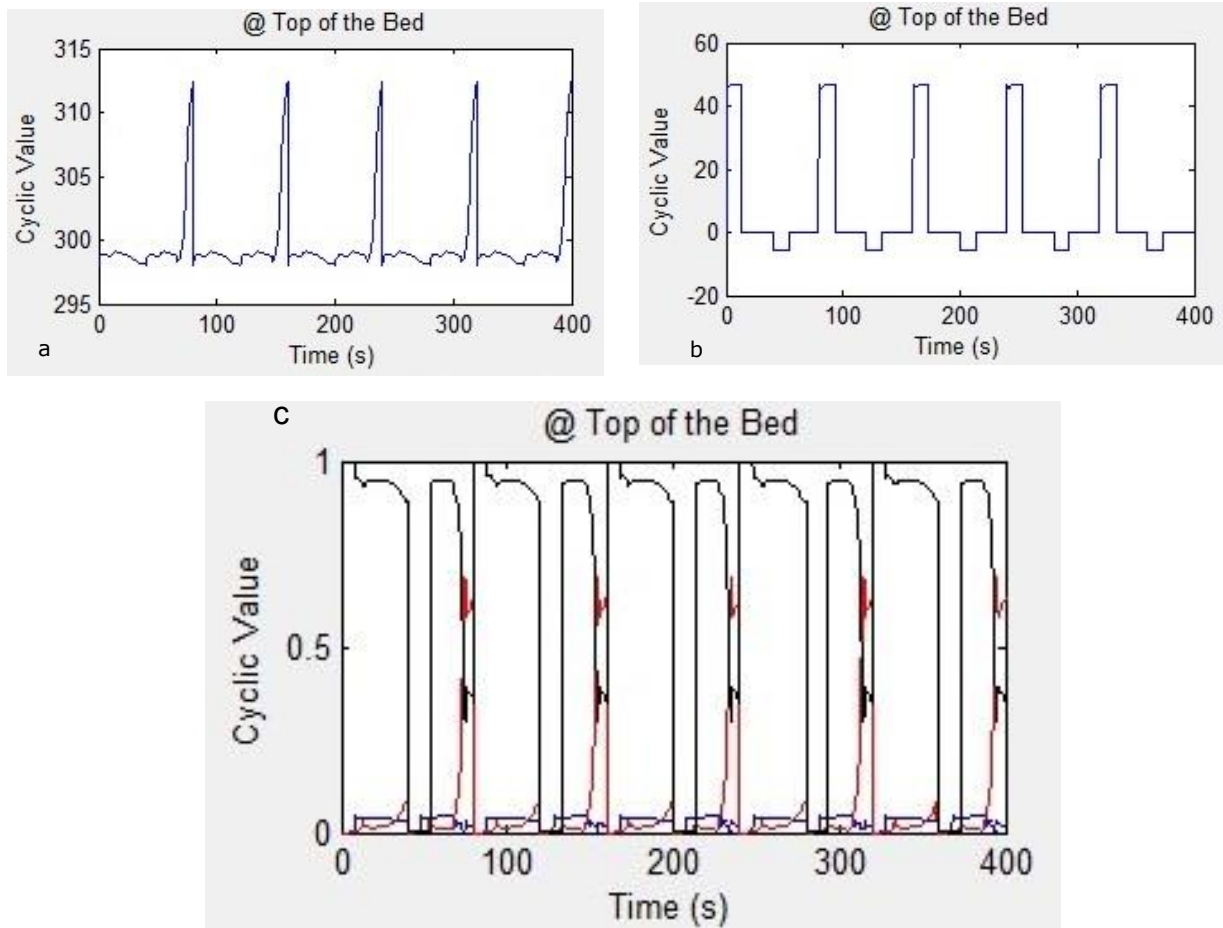


Figure 3 Online simulation results of TB-PSA-SS, (a: temperature (k); b: flowrate (Ln/min); c: pressure (bar)).

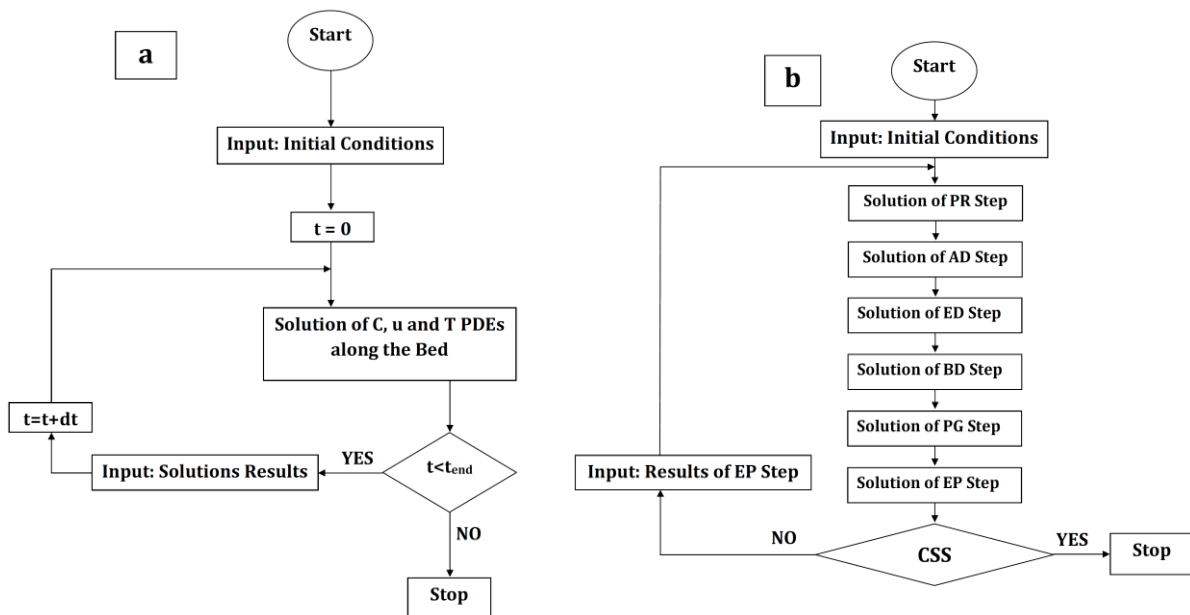


Figure 4 Schematic diagram of mathematical solution algorithm of CSS in TB-PSA-SS, (a: each step; b: CSS).

4. Conclusions

Accurate and applicable software (TB-PSA-SS) for numerical simulation of two-bed pressure swing adsorption processes (PSA) is presented. This software is designed in a way to simulate the dynamic behavior of three-component gaseous mixture adsorption, which uses the axially dispersed plug flow model as the fluid flow model, Langmuir-Freundlich adsorption model as the thermodynamic model and linear driving force (LDF) model for the mass transfer model. We suppose to mention some advantages and properties of this software: 1. It can be used easier in contrast to MATLAB code. 2. It is executable 3. There is no need to another software to run it like MATLAB or C++. 4. Onboard data Import. Properties: 1. Three-component feed analysis 2. 5th order Runge-Kutta scheme is used to solve partial differential equations. 3. Software simulation results save in txt format. 4. Online cyclic diagrams are drawn after running the program.

Nomenclature

A_w	wall cross-sectional area (cm^2)	PP	providing purge step
AD	adsorption step	Pr	reduced pressure, (---)
B	L-F parameter (atm^{-1})	PG	purge step
BD	blow down step	PR	pressurization step
cp_g	gas heat capacities ($cal/g.K$)	q	amount adsorbed (mol/g)
cp_s	pellet heat capacities ($cal/g.K$)	q^*	equilibrium amount adsorbed (mol/g)
cp_w	wall heat capacities ($cal/g.K$)	q_m	saturated amount adsorbed (mol/g)
D_L	axial dispersion coefficient (cm^2/s)	R	gas constant ($cal/mol.K$)
ED	equalization to depressurization step	R_p	radius of the pellet (cm)
EP	equalization to pressurization step	R_{Bi}	inside outside radius of the bed (cm)
h_i	internal heat-transfer coefficient ($cal/cm^2.K.s$)	R_{Bo}	outside outside radius of the bed (cm)
h_o	external heat-transfer coefficient ($cal/cm^2.K.s$)	t	time (s)
ΔH^-	average heat of adsorption (cal/mol)	T	gas phase temperature (k)
ID	idle step	T_{atm}	temperature of the atmosphere (K)
k	parameter for the LDF model	T_w	wall temperature (K)
K_L	axial thermal conductivity ($cal/cm.s.K$)	u	interstitial velocity (cm/s)
L	bed length (cm)	y_i	mole fraction of species i in gas phase
P	total pressure (atm)	Z	axial distance (cm)

Greek Letters

α	particle porosity
ϵ	voidage of the adsorbent bed
ϵ_t	total void fraction
ρ_g	gas density (g/cm^3)
ρ_p	pellet density (g/cm^3)
ρ_B	bulk density (g/cm^3)
ρ_w	wall density (g/cm^3)

Subscripts

B	bed
i	component i
p	pellet
g	gas phase
s	solid
w	wall

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