Object Oriented Modeling of Single and Multi-Bed Pressure Swing Adsorption Processes using OpenModelica

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Abstract

Pressure Swing Adsorption has been implemented to produce pure oxygen from air. Its model is solved using the methods of finite difference and orthogonal collocation on finite elements. Discrete events of this process are modelled using state graphs. Solution to the PSA process using a single bed is presented. With two beds, it is shown that it is possible to produce oxygen continuously. All of these have been done using OpenModelica, and the code is released as open source.
Keywords:Pressure swing adsorption, state graph, Open Source, High purity oxygen production

1 Introduction

Pressure Swing Adsorption (PSA) is a technology employed for separations and purification of gases. PSA operates on the basis of preferential adsorption of some gases on adsorbents, such as molecular sieves. Pressure is varied across the operations, and hence the name. (Skarstrom 1959) used the PSA process first time to enrich oxygen and nitrogen in a heatless drier. Skarstrom invented a two-bed cycle for the PSA to produce oxygen with pressure equalization step using zeolite 13X adsorbent. The PSA process has been widely utilised from then on ruthven1984principles. (Hassan, D. Ruthven, and Raghavan 1986) proposed a simple dynamic model to produce oxygen from the PSA process, It is based on linear rate of mass transfer and used Langmuir adsorption equilibrium equations. They further assumed that pressure remained constant during adsorption and desorption steps. (Farooq, D. Ruthven, and Boniface 1989) also introduced a kinetically controlled dynamic model for the Oxygen-PSA process. The advantage of kinetically controlled model is that mass transfer effects and axial dispersion are easy to calculate. (Farooq and D. Ruthven 1990) developed a linear driving force model and used carbon molcular sieves. The four steps used for the PSA cycle consists of:

1. Pressurisation.
2. Adsorption
3. Blow-down.
4. Purging with product.

PSA process is greatly influenced by design parameters such as bed length, time for each step viz. pressurization, feed, blowdown and purge. It is also influenced by feed and purge flow rates, production rate, temperature, pressure, etc. So it is imperative to obtain optimum amount of process variables.

In this work a general purpose OpenSource simulator for PSA is developed on the top of OpenModelica. Partial differential equations governing PSA model are solved numerically by developing generalized functions for finite difference and orthogonal collocation on finite elements techniques. Use of state-graphs enable visual and hence error-free implementation of the switching operation.

2 State-Graph Library in OpenModelica

StateGraph is an inbuilt library in OpenModelica which is used here for control applications. It is an upgraded finite state machine based on JGrafchart method that utilises Modelica feature of "action" language. The StateGraph has similar modeling capabilities as that of StateCharts with improved features. Main elements of a StateGraph are Steps and Transitions, as shown in Fig. 1.

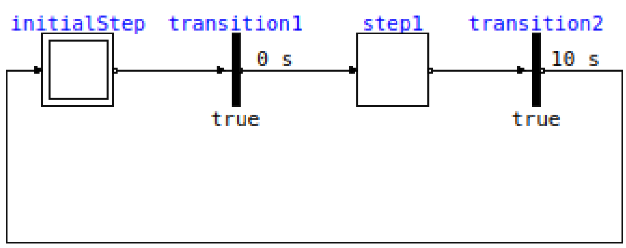

Figure 1. Steps and Transition blocks in StateGraphs

We explain the concept of StateGraph now, as it is used extensively in this wrok. Steps are represented by square boxes and transition by rectangles. Initial step is represented by double square boxes. Possible states of the StateGraphs are represented by Steps. A state can be changed by the use of Transitions. If a step is active then associated Boolean variable is true and becomes false otherwise. A transition fires when condition associated with it becomes true leading to input step to change to inactive state and output step becomes active.

In Fig. 1 the wait time for transition is given as 0 sec and set true. Therefore at time 0 tranistion1 fires and step1 becomes active leading to initialStep become inactive. The wait time for transition2 is 10 sec. Therefore, transition2 fires after 10 sec of transition1 leading step1 to be inactive and initialStep becomes active and cycle continuous.

3 PSA Process

Pressure Swing Adsorption (PSA) is based on the preferential adsorption of some gases on adsorbents, such as molecular sieves. In general, PSA includes four-steps:

1. Pressurization: Pressure plays a crucial role in adsorption of gases on solids. A gas is particularly adsorbed on the solid bed at high pressure according to bed characteristics and desorbed at lower pressure. The first step is pressurization where bed is pressurized with high pressure inert gas. This helps in avoiding sudden shock during the high pressure feed inlet step.

2. Adsorption or Production: This step is the production process wherein the feed is introduced from the bottom of the bed. Some components of the gas mixture preferentially get adsorbed according to the adsorbate and adsorbent characteristics, thereby enabling the separation of gases. Pure product gas is taken out from the other end.

3. Counter-Current Blowdown: When the bed gets saturated with adsorbed gases, whatever feed comes in it goes as it is to the outlet. No more separation is now possible. So bed needs to be regenerated by exposing it to atmosphere/low pressure. Due to pressure difference components flow out of the bed.

4. Counter-Current Purge: Pure product gas at low pressure is passed counter current from the top of the bed. Desorption takes place and bed gets regenerated for using in next cycle. fig:O2Prod demonstrates this for oxygen production.

4 Numerical Solution of Adsorption in a Fixed Bed

In this section, we will outline the model for adsorption in a fixed bed, and the numerical methods to solve them.

We assume that the concentration gradients are mainly along axial direction because of high aspect ratio of the bed. Linear driving force for mass transfer is assumed. The concentration and the mole fraction of components in the gas stream are given by

$$C_j = \frac{Y_j P}{RT_g} \tag{1}$$

where, P and T_g are the total pressure and temperature of gas stream, respectively, C_j and Y_j are the concentration and mole fraction of component j.
Langmuir Model:

$$\frac{\partial \bar{q}_j}{\partial t} = -K_{L,j}(q_j^* - \bar{q}_j) \tag{2}$$

Component Mass Balance:

$$\varepsilon \frac{\partial C_j}{\partial t} + \frac{\partial u C_j}{\partial Z} = \varepsilon D_{ax}\left(\frac{\partial^2 C_j}{\partial^2 Z}\bigg|_{z=0^-}\right) - (1-\varepsilon)\rho_P \frac{\partial \bar{q}_j}{\partial t} \tag{3}$$

Bulk Mass Balance:

$$\varepsilon \frac{\partial C_T}{\partial t} + \frac{\partial u C_T}{\partial Z} = \varepsilon D_{ax}\left(\frac{\partial^2 C_T}{\partial^2 Z}\right) - \sum(1-\varepsilon)\rho_P \frac{\partial \bar{q}_j}{\partial t} \tag{4}$$

Initial Conditions:
$t = 0$:

$$C_j(Z,0) = \bar{q}_j(Z,0) = 0 \tag{5}$$

Boundary Conditions:
Counter-current Pressurization Step:
$Z = L$:

$$\varepsilon D_{ax}\left(\frac{\partial C_j}{\partial Z}\right)\bigg|_{Z^+} = -u(C_j\big|_{Z^-} - C_j\big|_{Z^+})$$

$Z = 0$

$$\left(\frac{\partial C_j}{\partial Z}\right)\bigg|_{Z^-} = 0 \tag{6}$$

Production Step:
$Z = L$:

$$\varepsilon D_{ax}\left(\frac{\partial C_j}{\partial Z}\right)\bigg|_{Z^+} = -u(C_j\big|_{z^-} - C_j\big|_{z^+}) \tag{7}$$

$Z = 0$:

$$\left(\frac{\partial C_j}{\partial Z}\right)\bigg|_{Z^-} = 0 \tag{8}$$

Counter-current Blowdown Step:
$Z = 0$:

$$\left(\frac{\partial C_j}{\partial Z}\right)\bigg|_{Z^-} = 0 \tag{9}$$

Counter-current Purge Step
$Z = L$:

$$\varepsilon D_{ax}\left(\frac{\partial C_j}{\partial Z}\right)\bigg|_{Z^+} = -u(C_j\big|_{Z^-} - C_j\big|_{Z^+})$$

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$Z = 0$

$$\left(\frac{\partial C_j}{\partial Z}\right)\Big|_{Z^-} = 0 \tag{10}$$

Table 1. Variables used in Fixed Bed Model

C_j	Concentration of species (mol/m^3)
P	Total pressure (bar)
R	Gas Constant
Tg	Temperature of gas (K)
$\bar{q}_j$	Equilibrium Concentartion of species
q_j^*	Concentration of species in solid bed
ε	Porosity
u	Velocity(m/s)
D_{ax}	Axial dispersion coefficient
ρ_p	Density of particle (kg/m^3)
C_T	Bulk gas concentration

The easiest method to solve the above set of equations is the finite difference method, using which, the PDE is converted into ordinary differential equations (ODEs), which are solved using an integrator, such as DASSL. In this work, we divided the bed into 10 intervals of equal length.

Orthogonal collocation on finite elements is in general a faster method to solve the PDEs. We divide the entire length of the bed into three short subsections (0-0.3, 0.3-0.7, 0.7-1), which allows us to use a low order polynomial to approximate the solution. This in turn reduces the undesirable oscillatory phenomenon. Legendre third degree polynomials are used in this work to approximate the solution. It is possible to find the coefficients of the polynomials in the three subsections using appropriate continuity conditions. The resulting ODEs are solved using DASSL.

5 Modelling Pressure Swing Adsorption

In this section, we concentrate on operating the fixed bed in four different modes, namely, pressurization, production, blowdown, and purge. We begin with the example of oxygen production from air. The OpenModelica code developed in this work is available at (NikhilOM 2021).

5.1 Example: Oxygen Production from Air using PSA

In this section, we devote our attention to the process of producing high purity oxygen by separating it from nitrogen in air. Mathematical equations that describe the underlying adsorption process have already been presented in Sec. 4. The four step process for fixed bed adsorption is shown in Fig. 2.

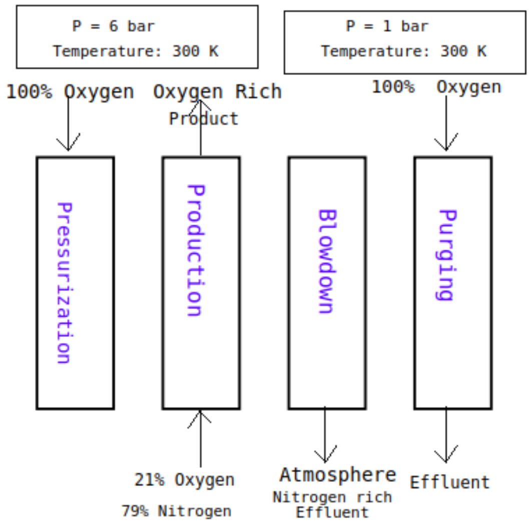

Figure 2. Four step adsorption process for fixed bed adsorption

The fixed bed is pressurized with pure O_2 at high pressure of 6 bar absolute pressure at 300 K. Feed is a mixture of N_2 and O_2 with 79% and 21% composition respectively is passed from the opposite end to that of pressurization. Here the adsorption of N_2 takes place and pure O_2 comes out till the bed is saturated. Next step after bed gets saturated is blowdown operation where bed is exposed to low pressure atmosphere and due to pressure difference adsorbed gases comes out after desorption and effluent is rich in N_2. During the purging operation pure O_2 is passed counter currently at low pressure of 1 bar and bed is regenerated with effluent coming out from the other end. The time intervals for pressurization, production, blowdown, and purging are taken respectively as 30%, 20%, 30% and 20% of the cycle time, as suggested by (Douglas M Ruthven 1984).

5.2 Implementing Discrete Events using State-Graphs

Depending on the four modes of operating the fixed bed, an appropriate model has to be solved. The model selection for each of the four modes is achieved by opening/-closing valves using using state-graphs, an inbuilt library in OpenModelica. Fig. 3 shows the diagram view of PSA process for the fixed bed adsorber for O_2 production in OpenModelica. It shows process steps are actuated by valves which in turn are modeled separately using State-Graphs shown in Fig. 4. The valve connected to pressurization unit is opened when boolean expression associated with it is true. As shown in Fig. 3 boolean expression connected to pressurised section becomes true when step is active which is evident from Fig. 4 that it happens at time 0. The same logic is applicable to opening and closing of valves associated with other steps.

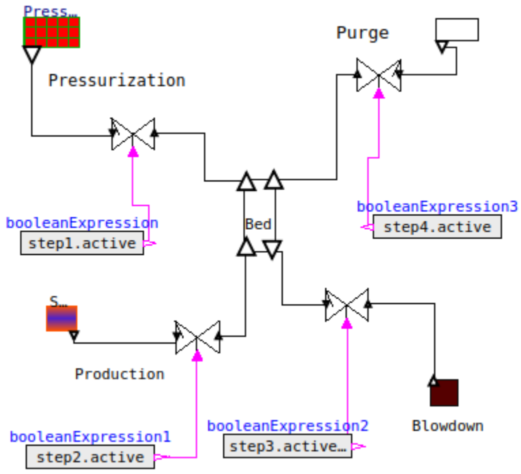

Figure 3. Diagram view of the four step PSA process in OpenModelica. Boolean expressions are activated as per the StageGraph in Fig. 4.

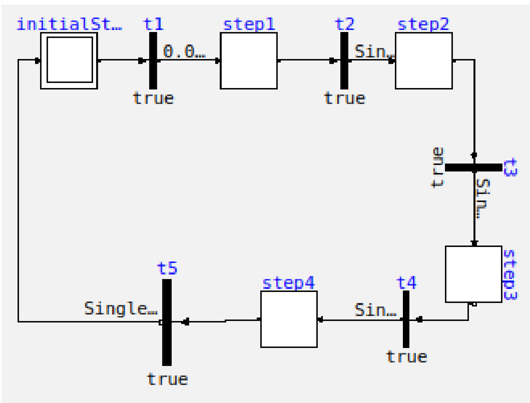

Figure 4. Steps Implementation of Fixed Bed Adsorber using StateGraphs. Variables step1, step2, step3 and step4 are activated respectively at (0.3,0.2,0.3,0.2) × (cycle time)

6 Simulation of Single Bed PSA Process

The parameters used for O_2 production in this work are given in Table 2 and Table 3.

For pressurization, pure O_2 at high pressure of 6 bar is passed for 30% of cycle time. During the production step feed air which is a mixture of N_2 and O_2 is supplied at the other end. The feed step takes place for 20% of the cycle time. For blowdown operation, the bed is exposed to atmosphere for 30% of the cycle time. During the purge operation, pure O_2 is again passed counter-currently at a low pressure of 1 bar for 20% of the cycle time. These values are tabulated in Table 4.

Fig. 5 shows the mole fraction of N_2 at outlet i.e at the point at each time. Cycle time is taken as 1100s. One can see from the figure that no N_2 comes out at time interval 600-780s, as the mole fraction of N_2 during this interval is zero. During this interval, pure oxygen is produced, as one

Table 2. Input Parameters

Particle Dia.	0.0038 m
Void Fraction, ε	0.5418
Particle Density, ρ	600 Kg/m^3

Table 3. Properties of Adsorbent

Species	Max. Adsorbed Conc. q_m	b_0 Pa^{-1}
N_2	14	4.96e-10
CO_2	7.90	1.55e-11

Table 4. Step Time for O_2 Production

Steps	Time
Pressurization	330 sec
Production	220 sec
Blowdown	330 sec
Purge	220 sec

can see from the O_2 mole fraction profile, given in Fig. 6. This process is repeated at other time intervals also, as can be seen from these figures.

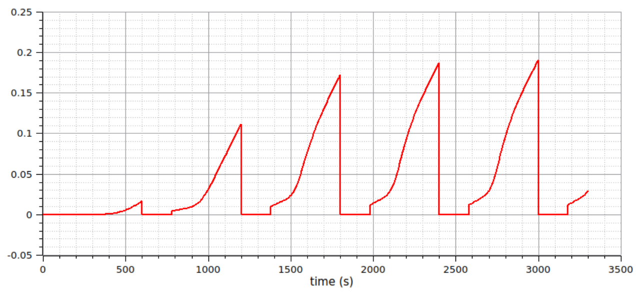

Figure 5. Mole Fraction of N_2 at outlet point

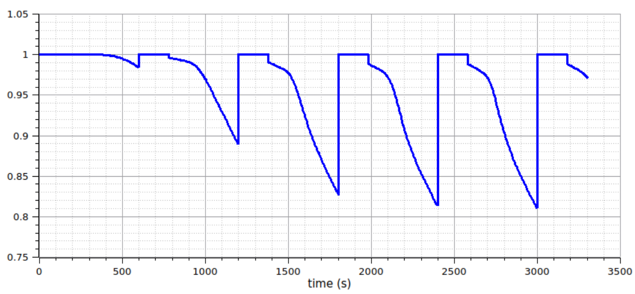

Figure 6. Mole Fraction of O_2 at outlet point

Using single bed adsorber pure oxygen can be obtained but the supply of pure Oxygen in the product is not continuous because the bed needs to be regenerated after saturation. One way to address this difficulty is to employ more

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beds.

7 Simulation of two bed PSA process

In this section, we show that it is possible to produce O_2 continuously with the help of two fixed beds. When product is taken out from a bed the other bed remains in the regenerated phase and vice-versa. Each of the two beds is operated exactly as described in the previous section.

The four step process for oxygen production using two beds of adsorbers is shown in Fig 7.

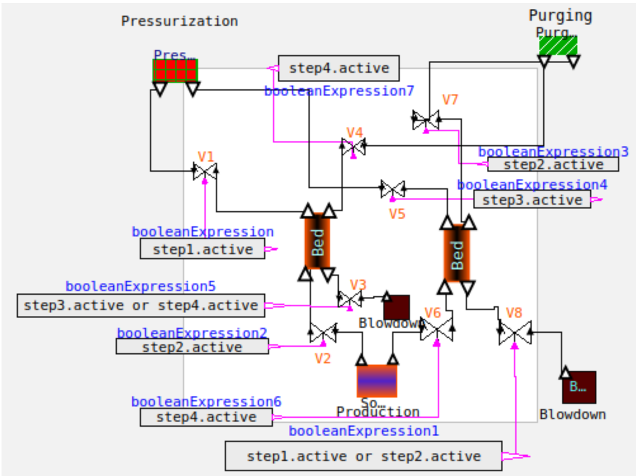

Figure 7. Multi-Cylinder adsorber for O_2 production

The operation of multi cylinder adsorber is described in Table 5.

Table 5. Four step process for multi cylinder bed

Step	Open valve	Bed-1	Bed-2
1	V1, V8	Pressurization	Blowdown
2	V2, V7, V8	Production	Purging
3	V3, V5	Blowdown	Pressurization
4	V3,V4 V6	Purging	Adsorption

Recall that we used the StateGraph in Fig. 4 for the single bed operation. The same StateGraph works for the two bed operation as well. The only difference is that now more than one valve is operated when a Boolean operation is active, as shown in Table 6.

Table 6. Steps Time for CO_2 Capture

Steps	Time
Pressurization	30 % of cycle time
Production	20 % of cycle time
Blowdown	30 % of cycle time
Purge	20 % of cycle time

The mole fraction of O_2 produced by the two bed PSA process is given in Fig 8. Blue line indicates the oxygen production in one bed, and the red line corresponds to that in the other bed. One can see that the oxygen mole fraction is almost 1 at all times.

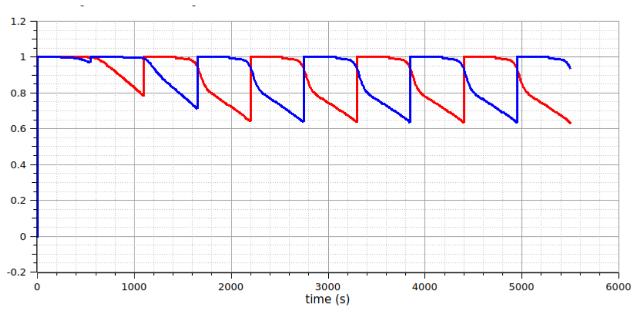

Figure 8. Mole fractions of O_2 at outlet of both beds for 1100 seconds

8 Conclusion

A model for PSA has been implemented and solved using the open source modeling and simulation environment OpenModelica. The object oriented modeling capability has enabled easy extension of a single bed PSA to multi-bed processes. The transitions occurring in PSA are implemented through the inbuilt library StageGraph in OpenModelica. As it is a visual method of programming, it is natural for engineers, and hence results in error-free coding. As the StateGraph capability is inbuilt, it results in error-free implementation as well.

Commercial software that is capable of modeling niche operations, such as PSA, can be prohibitively expensive to students, and to small and medium scale enterprises. As a result, this population may not have access to such important technologies. We are happy to partially address this issue by releasing our code as open source Code. We also believe that this is another initiative in the direction of collaborative content creation, and improving the employability of students, as articulated by (Nayak et al. 2019).

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