

# NUMERICAL STUDY OF ARGON EFFECT ON NITROGEN SEPARATION FROM AIR BY PRESSURE SWING ADSORPTION

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**ABSTRACT:** A mathematical model was used to design four modes of two-bed pressure swing adsorption (PSA) process to investigate argon presence in the feed mixture. The effect of operating parameters such as cycle time, pressure equalization, adsorption pressure, and purging flow rate was investigated. The model was validated with experimental data of nitrogen separation from the air by a single bed adsorber on carbon molecular sieve (CMS). A good agreement with experimental data is obtained. In the PSA process, higher purity of nitrogen (99.7%) was detected by mode 4 when the feed mixture was free of argon (O<sub>2</sub>: 21%, N<sub>2</sub>:79%). While the nitrogen purity was only 98.0% in the state of argon presence in the feed mixture (O<sub>2</sub>: 21%, N<sub>2</sub>: 78%, Ar: 1%). The results showed that the cycle time had insignificant effect whereas the pressure equalization and purging at low vacuum pressure had a significant effect on the process performance.

**ABSTRAK:** Model matematik digunakan bagi membina empat mod terdiri daripada tekanan dua-turus proses penyerapan buai (PSA) bagi menyiasat kehadiran argon dalam campuran pakan. Kesan parameter beroperasi seperti masa kitaran, penyamaan tekanan, tekanan penyerapan, dan kadar aliran penyingkiran disiasat. Model matematik tersebut disiasat melalui data eksperimen pemisahan nitrogen dari udara melalui penyerapan turus tunggal pada penapis molekular karbon (CMS). Data eksperimen yang bagus diperolehi. Dalam proses PSA, mod keempat menghasilkan ketulenan nitrogen (99.7%) lebih tinggi apabila campuran pakan bebas argon (O<sub>2</sub>: 21%, N<sub>2</sub>:79%). Sementara itu, ketulenan nitrogen hanya 98.0% apabila terdapat kehadiran argon dalam campuran pakan (O<sub>2</sub>: 21%, N<sub>2</sub>: 78%, Ar: 1%). Kajian menunjukkan masa kitaran memberi kesan tidak signifikan sementara penyamaan tekanan dan penyingkiran pada tekanan vakum rendah mempunyai kesan signifikan terhadap prestasi proses.

**KEYWORDS:** *nitrogen separation; PSA; argon; model simulation*

## 1. INTRODUCTION

Gaseous nitrogen is used extensively in many industries such as vessel inerting applications, electronics, metals, and food industries due to its inert properties [1]. A variety of separation processes are used to produce commercial nitrogen such as cryogenic distillation, adsorption separation, and membrane separation processes. PSA is one of the most important process in the field of gas separation [2-4]. A carbon molecular sieve

(CMS) is used as an adsorbent for nitrogen separation from air due to the difference in the kinetic adsorption of oxygen and nitrogen [5-7]. Since oxygen is faster than nitrogen to diffuse into the CMS, a kinetic selectivity is created, which allows reaching nitrogen purities as high as 99.999%. The demand for high nitrogen purity, over 99%, in a low and medium amount in the industrial sector has urged a lot of companies to produce nitrogen from atmospheric air by PSA process [8]. Zeolite X-type and perovskite-type ceramic were used as adsorbents instead of the CMS sieve for nitrogen separation from air at high pressure [9-12].

In the last decades, the PSA process was investigated experimentally and theoretically in many studies [13,14]. For instance, a simple linear driving force (LDF) model was created to simulate a single bed PSA process for nitrogen separation from the air on CMS. The feed mixture was assumed to be (O<sub>2</sub>: 21%, and N<sub>2</sub>:79%) [15]. The effect of bed length and pressurizing rate on the single bed PSA performance was studied carefully. The higher performance of the process was observed with a bed length over 1.3 m. The effect of the adsorption/desorption rate constants of oxygen on the nitrogen separation was evaluated through a simulation process and found that the purity varied significantly with cycle time [8,16]. Operating parameters such as feed flow, purge flow, cycle time, adsorption pressure, and bed length on the PSA process performance was studied experimentally and theoretically [17]. Higher purity of nitrogen was observed at short adsorption time. No significant effect of adsorption pressure over 4 bar on the process performance was observed. About 97.6% of nitrogen purity was detected using atmospheric air as a feed [2,3]. The purity was improved from 96% to over 99% by adding a deoxo reactor to the PSA process. The feed mixture only consisted of oxygen and nitrogen [18].

Many previous studies assume that the feed mixture only consists of O<sub>2</sub> and N<sub>2</sub>, but real air consists of argon as well. So, the main objective of this study is to investigate the effect of argon presence in the feed mixture and operating parameters on the nitrogen purity. A mathematical model is introduced to study the nitrogen separation from the air by single bed adsorber on a CMS sieve. Then, it is employed to design four configurations of the two-bed PSA process to deeply investigate the process and compare the four modes.

## 2. MODELING AND SIMULATION

A theoretical study is employed to investigate the nitrogen separation from atmospheric air by PSA process. The numerical study was applied to the following processes:

- a) Single bed adsorber to study the breakthrough time.
- b) Two-bed PSA process with the four different configurations as shown in Table 4.

The first design of the PSA process is represented by the Skarstrom cycle, which involved four steps: pressurizing, producing, depressurizing, and purging steps. Different modifiers are added such as purging by vacuum pump, pressure equalization, and product pressurizing, to improve the performance of the PSA process.

The numerical study of the PSA process was carried out using a simulation program. Finite difference method (FDM) is employed, and axial dimension is discretized into 50 nodes. The purity of oxygen or nitrogen is used as an indication of the process performance. The following assumptions are considered in the numerical study:

- 1- Feed mixture assumed to be (O<sub>2</sub>:21%, N<sub>2</sub>:78%, Ar:1%, and O<sub>2</sub>:21%,N<sub>2</sub>:79%).

- 2- Ideal gas law is applied.
- 3- Isothermal system.
- 4- The flow pattern is described by the axial dispersion plug flow model.
- 5- Radial concentration is neglected.
- 6- Mass Transfer transport is described by a linear driving force (LDF).
- 7- Adsorption equilibrium is fitted with the Langmuir equation.
- 8- Pressure drop along the bed is represented by the Darcy equation.

Overall mass balance:

$$-D_L \frac{\partial^2 c_i}{\partial z^2} + \frac{\partial C}{\partial t} + \frac{\partial(uC)}{\partial t} + \sum_{i=1}^n \rho_p \left( \frac{1-\varepsilon}{\varepsilon} \right) \frac{\partial \bar{q}}{\partial t} = 0 \quad (1)$$

Component (i) mass balance:

$$-D_L \frac{\partial^2 c_i}{\partial z^2} + \frac{\partial(uc_i)}{\partial z} + \frac{\partial c_i}{\partial t} + \rho_p \left( \frac{1-\varepsilon}{\varepsilon} \right) \frac{\partial \bar{q}}{\partial t} = 0 \quad (2)$$

Boundary conditions of each step of the PSA process are presented in Table 1. The boundary conditions of well-known Danckwerts are applied [19]. The adsorption isotherm and adsorption rate parameters of N<sub>2</sub>, O<sub>2</sub>, and Ar on CMS are presented in Table 2. The operating parameters of the single bed adsorber are presented in Table 3. The operation parameters of other modes of PSA process are presented in Table 4.

Table 1: Applied boundary conditions in the simulation process.

Cycle step	Concentration (c <sub>i</sub> )	Velocity (u)
Pressurizing (Pre)	$-D_L(\partial c_i / \partial z) _{z=0} = u(c_i _{z=0-} - c_i _{z=0+})$ $(\partial c_i / \partial z) _{z=L} = 0$	$u _{z=0} = u_{\text{feed}}$ $u _{z=L} = 0$
Adsorption (Ads)	$-D_L(\partial c_i / \partial z) _{z=0} = u(c_i _{z=0-} - c_i _{z=0+})$ $(\partial c_i / \partial z) _{z=L} = 0$	$u _{z=0} = u_{\text{feed}}$
Depressure- Equalization (DepEqu)	$-D_L(\partial c_i / \partial z) _{z=0} = 0$ $-D_L(\partial c_i / \partial z) _{z=L} = 0$	$u _{z=0} = 0$
Depressurizing (Dep)	$D_L(\partial c_i / \partial z) _{z=0} = 0$ $-D_L(\partial c_i / \partial z) _{z=L} = 0$	$u _{z=L} = 0$
Purging (Pur)	$-D_L(\partial c_i / \partial z) _{z=L} = u(c_i _{z=L+} - c_i _{z=L-})$ $-D_L(\partial c_i / \partial z) _{z=0} = 0$	$u _{z=L} = u_{\text{purge}}$
Pressure-Equalization (PreEqu)	$-D_L(\partial c_i / \partial z) _{z=0} = u(c_i _{z=0-} - c_i _{z=0+})$ $(\partial c_i / \partial z) _{z=L} = 0$	$u _{z=0} = 0$

Initial conditions:

$$c_i(z, 0) = c_0; \quad q_i(z, 0) = q_i^*$$

Ideal gas law:

$$\frac{P}{RT} = \sum_{i=1}^n c_i \quad (3)$$

The adsorption rate is described by the LDF equation with concentration-dependent diffusivity:

$$\frac{\partial \bar{q}_i}{\partial t} = \omega_i (q_i^* - \bar{q}_i), \quad \omega_i = \frac{15D_{ei}}{r_c^2} \quad (4)$$

Where:  $D_{ei}/r_c^2 = CP_r^{0.5}(1 + B_i P_i)^2$

The LDF coefficient ( $\omega_i$ ) has been estimated from the fitting between the mathematical model and experimental data of single bed adsorber from the literature survey. The predicted values are presented in Table 2.

The adsorption isotherm for multi-components (oxygen, nitrogen, and argon) are predicted by the Langmuir equation to the n-component mixture:

$$q_i = \frac{q_{mi} B_i P_i}{1 + \sum_{j=1}^n B_j P_j} \quad (5)$$

Where:  $q_{mi} = k_1 + k_2 * T$ , and  $B = k_3 \exp\left(\frac{k_4}{T}\right)$ ,

Table 2: Adsorption equilibrium and adsorption rate parameter [20].

Parameters	O <sub>2</sub>	N <sub>2</sub>	Ar
K <sub>1</sub> *10 <sup>3</sup> (mol/g)	5.817 × 10 <sup>-3</sup>	1.130 × 10 <sup>-2</sup>	9.556 × 10 <sup>-3</sup>
K <sub>2</sub> *10 <sup>5</sup> (mol/g)	-7.512 × 10 <sup>-6</sup>	-2.80 × 10 <sup>-5</sup>	-2.101 × 10 <sup>-5</sup>
K <sub>3</sub> *10 <sup>5</sup> (1/Kpa)	7.984 × 10 <sup>-6</sup>	30.89 × 10 <sup>-5</sup>	6.566 × 10 <sup>-5</sup>
K <sub>4</sub> (k)	1444	359.7	773.8
$\omega_i$ (s <sup>-1</sup> )	0.248	0.001	0.0071

Darcy's equation used to predict pressure drop:

$$-\frac{dP}{dz} = \frac{180\mu(1 - \epsilon)^2}{D_p^2 \epsilon^2} u \quad (6)$$

Where :  $u$  is the superficial gas velocity.

Table 3: Adsorbent and common parameters were used in the single bed process.

Adsorbent	CMS
Type	Pellet
Pellet density $\rho_p$ (kg/m <sup>3</sup> )	800
Bed voidage ( $\epsilon$ )	0.30
Adsorption bed	
Length (m)	1
Diameter (m)	0.0254
Ambient temperature (°C)	25
Adsorption pressure (bar)	7
Product flow rate (liter/min)	1

The performance of the PSA process is indicated by the purity and recovery of nitrogen according to the following equations:

$$Purity(N_2\%) = \frac{\text{amount of } N_2 \text{ produced during adsorption step in the product end}}{\text{amount of total product produced during adsorption step in the product end}} \quad (8)$$

$$Recovery(N_2\%) = \frac{\text{amount of } N_2 \text{ produced during adsorption step in the product end}}{\text{amount of } N_2 \text{ fed during pressurizing, and adsorption steps in the feed end}} \quad (9)$$

Table 4: Operated conditions of the four modes of the PSA process.

The PSA Modes	Pressure (bar)	Product flowrate (liter/min)	Purge flowrate (liter/min)	Vacuum purging (bar)	Cycle step time (sec)
					Pre - Ads - Dep - Pur
2-bed 4-step (mode 1)	2-9	0.1-5	1-6	No	5 - 20 - 5 - 20
					5 - 30 - 5 - 30
					5 - 40 - 5 - 40
					5 - 50 - 5 - 50
					5 - 60 - 5 - 60
					5 - 70 - 5 - 70
2-bed 4-step with vacuum purging (mode 2)	7	0.1-1	1-3	Yes	Pre - Ads - Dep - VacPur
					5 - 80 - 5 - 80
2-bed 6-step with equalization pressure (mode 3)	7	0.1-1	1-6	No	Pre - Ads - DepEq - Dep - Pur - PreEq
					5 - 80 - 5 - 5 - 80 - 5
2-bed 6-step with equalization pressure and vacuum purging (mode 4)		0.1-1	1-3	Yes	Pre - Ads - DepEq - Dep - VacPur - PreEq
					5 - 20 - 5 - 5 - 20 - 5
					5 - 30 - 5 - 5 - 30 - 5
					5 - 40 - 5 - 5 - 40 - 5
					5 - 50 - 5 - 5 - 50 - 5
					5 - 60 - 5 - 5 - 60 - 5
					5 - 70 - 5 - 5 - 70 - 5
					5 - 80 - 5 - 5 - 80 - 5
5 - 90 - 5 - 5 - 90 - 5					
5 - 100 - 5 - 5 - 100 - 5					

### 3. RESULTS AND DISCUSSION

#### 3.1 Single Bed Adsorber

The breakthrough curve of oxygen at the product end of the single bed adsorber for nitrogen separation from the air on CMS is shown in Fig. 1. The effluent flow rate is 1

liter/min. The breakthrough time occurred at 100 s. Thereby, the oxygen purity gradually increased until it reached a stable purity of about 20%. The mass transfer zone (MTZ) is very wide due to the effect of axial dispersion during the pressurizing and producing steps. The predicted results are in good agreement with experimental data obtained by Abdel-Rahman [3].

Figure 2 represents the effect of product pressurizing pressure on the breakthrough time and the amount of nitrogen produced. A little improvement in the breakthrough time and in the amount of nitrogen produced was noticed. That is because the adsorption isotherm of oxygen and nitrogen are closer to each other on the CMS at equilibrium state. So increasing in the product pressurizing pressure leads to increase in the partial pressure of nitrogen in the bed and the most porosities of the adsorbent (CMS) are filled by nitrogen. Therefore, little increases in the breakthrough time may be attributed to increases in adsorbent capacity with pressure and decreased axial dispersion effects.

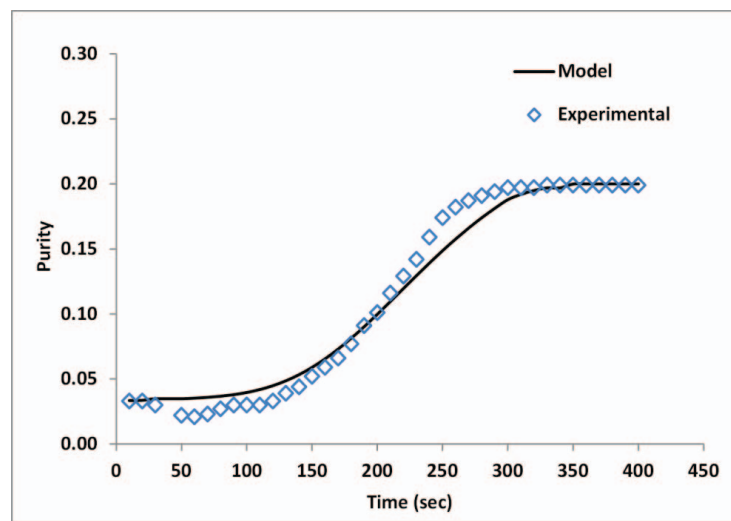


Fig. 1: Fitting between the predicted results and experimental data of oxygen breakthrough curve in the product end of single bed adsorber.

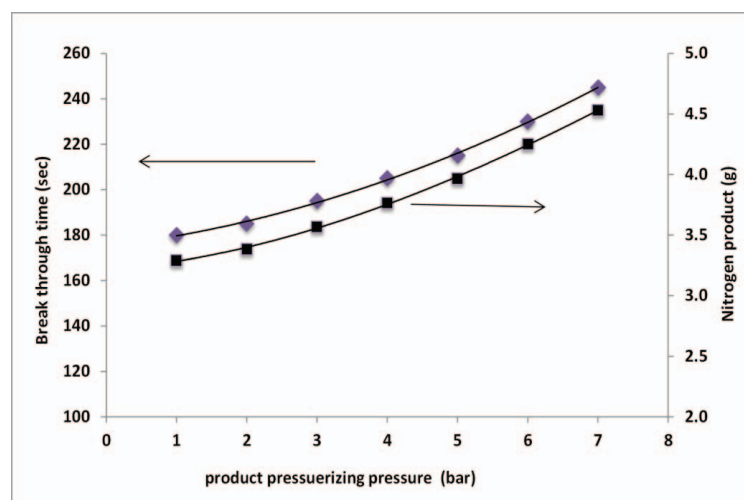


Fig. 2: Effect of product pressurizing pressure on the breakthrough time and amount of produced nitrogen in single bed adsorber.

## 3.2 Two Bed PSA Process

### 3.2.1 Effect of the Ternary Feed Mixture

Figure 3 represents the effect of the argon presence in the feed mixture on the performance of the 2-bed 6-step PSA process (mode 3) at 7 bar pressure, 80 s adsorption time, 1-4 liter/min purge flow rate, and 0.1 liter/min product flow rate. Higher purity of nitrogen, over 99% is observed in the state of a binary feed mixture ( $O_2/N_2$ ) than a ternary feed mixture ( $O_2/N_2/Ar$ ), where the maximum purity was about 95%. According to the LDF coefficient values, oxygen diffuses faster than nitrogen and argon through the CMS porosity, therefore the purity of nitrogen in the product end could not be higher than the purity of the PSA process with the binary feed mixture. Most studies obtained high purity of nitrogen, over 99% when they handled a binary feed mixture.

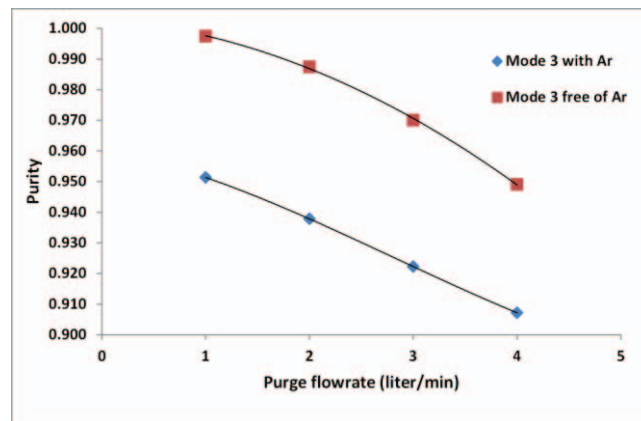


Fig. 3: Effect of argon presence in the feed mixture on the performance of mode 3 of PSA processes.

### 3.2.2 Effect of Adsorption Pressure

Figure 4 shows the effect of adsorption pressure (2-9 bar) on the product purity of 2-bed 4-step PSA processes (mode 2), at purge flow rate of 1 liter/min, product flow rate of 1 liter/min, and adsorption time of 40 s. The purity of nitrogen and argon are increased with increasing adsorption pressure, due to increase in the adsorption capacity of the CMS to adsorb more oxygen. The same trend is detected with the argon component. Only oxygen is adsorbed by CMS, therefore the purity of nitrogen in the product could not be higher due to the argon presence in the feed mixture.

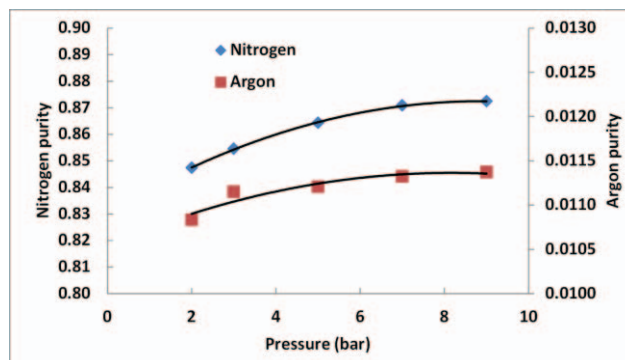


Fig. 4: Effect of adsorption pressure on the purity of the nitrogen and argon in the mode 2 of the PSA process.

### 3.2.3 Effect of Adsorption Time

Figure 5 shows the effect of adsorption time in the range of 40-250 s with two different feed mixtures, at adsorption pressure of 7 bar, purge flow rate of 1 liter/min, and product flow rate of 1 liter/min. Nitrogen purity increased with increasing adsorption time until 100 s and then decreased slightly or kept stable. Nitrogen separation on CMS is kinetically controlled. Increase in the adsorption time over 100 s leads to the system approaching an equilibrium state, causing decreases in the nitrogen purity or keeping it stable. At short adsorption time, the time is not enough to adsorb the whole oxygen molecule by CMS. Maximum uptake is obtained at nearly 100 s. Maximum purity (98%) is detected by mode 3 without argon presence in the feed mixture, while it dropped to 92% with argon presence in the feed mixture.

The production of nitrogen purity by mode 3 regardless of feed mixture components binary or ternary is higher than mode 1. This may be attributed to the effect of the pressure equalization step in mode 3, which contributed to reducing the axial dispersion effect during the pressurizing step. Moreover, the rapid diffusion of oxygen into the CMS led to the adsorption of oxygen rather than argon and nitrogen, where the diffusion rate constant of oxygen is higher than nitrogen and argon as shown in Table 2. CMS is a kind of adsorbent material with pore sizes in the range of 3-5 Å while the diameter of oxygen is (3.46 Å), diameter of nitrogen is (3.64 Å) and the diameter of argon is (3.43 Å). All these reasons lead to kinetic separation of air on CMS. Despite the smaller diameter of argon than other components, low partial pressure of argon in the feed mixture and small diffusion rate constant reduced argon diffusion in the state of the ternary feed mixture. This phenomenon was observed by Jee [20] when they used two ternary feed mixtures (O<sub>2</sub>/Ar/N<sub>2</sub>; 95:4:1 and 90:4:6 vol%) for gas separation on CMS. Nitrogen recovery increased with increasing adsorption time, where the product flow rate increased with increasing the adsorption time. The results are in a good agreement with LaCava [16], Farooq [21], and Mostamand [2].

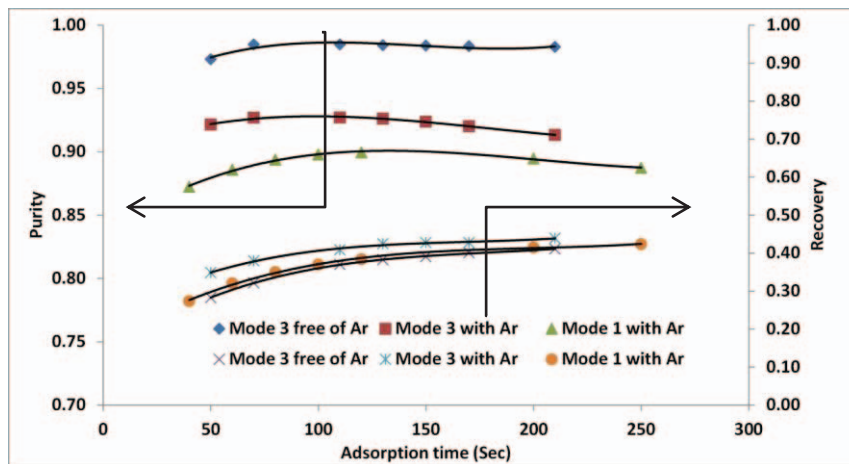


Fig. 5: Effect of the adsorption time on the performance of two modes of PSA process.

### 3.2.4 Effect of Purge Flowrate

Figure 6 shows the effect of purge flow rate for all modes of PSA process on the purity of nitrogen at adsorption time of 80 s, adsorption pressure of 7 bar, and product flow rate of 1 liter/min. In all modes, nitrogen purity was approximately kept constant or decreased slightly with increased purge flow rate until 2 liter/min, and it then decreased



dramatically. The gas used in the purging step is represented as part of the product flow rate during the adsorption step and is enriched with nitrogen. Increasing it over 2 liter/min causes an increase in vapor pressure of nitrogen, after displacing oxygen out of the bed and adsorbing it by CMS. So in the next cycle, nitrogen purity will inevitably drop, because most CMS porosity is filled with nitrogen during the purging step. In addition, both the depressurizing step and low purge flowrate (< 1 liter/min) were enough to expel adsorbed oxygen from CMS porosity. The most out of purge flow rate is observed at low purge flow rate. The results are in agreement with Farooq [21], and Abdel-Rahman [3], and in disagreement with Mostamand [2].

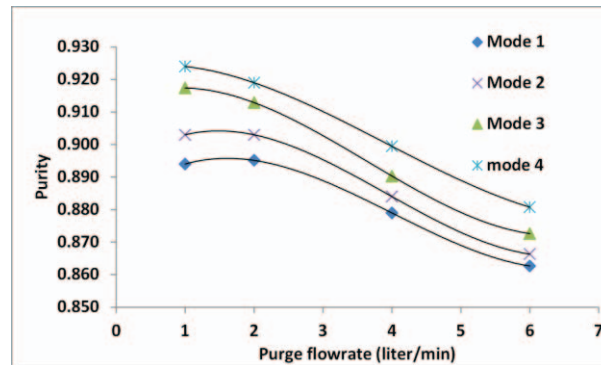


Fig. 6: Effect the purge flow rate on the four modes of the PSA process.

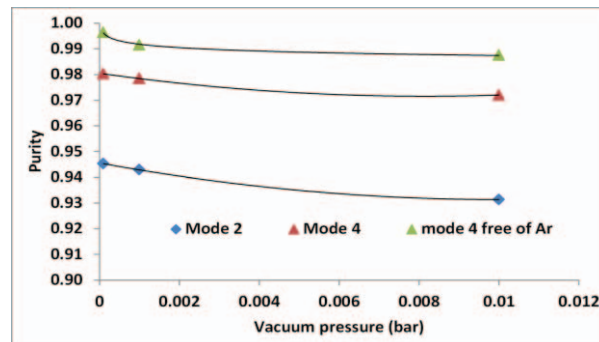


Fig. 7: Effect of vacuum pressure on the performance of two modes of the PSA processes.

### 3.2.5 Effect of Vacuum Pressure

Figure 7 shows the effect of vacuum pressure on the effluent nitrogen purity at adsorption pressure of 7 bar, purge flow rate of 1 liter/min, product flow rate of 0.1 liter/min, and adsorption time of 80 s. All processes have the same trend. High nitrogen purity is detected at a low vacuum pressure (0.0001 bar) and then decreased slightly with increasing vacuum pressure. Purging the adsorbent at low vacuum pressure has a significant effect to clean the adsorbent during the purging step. Increases of vacuum pressure lead to sufficient desorption of CMS to prepare it for the next cycle. Maximum purity, over 99% is observed by mode 4 with the binary feed mixture, while low purity of about 98% is observed with the same mode (mode 4) with the ternary feed mixture. The nitrogen purity produced by mode 4 with a feed mixture that is free of argon is higher than mode 4 with ternary feed mixture and mode 2. This may be attributed to the faster rate of diffusion of oxygen than nitrogen and argon on CMS, the presence of the pressure equalization step, and the purging step at low vacuum pressure, where they contributed to

improving the process performance. It is important to consider the argon presence in the feed mixture, and operation steps to design the PSA unit to produce high purity nitrogen from atmospheric air.

#### 4. CONCLUSIONS

The mathematical model of single bed adsorber is in good agreement with experimental data. The breakthrough time and amount of nitrogen product are increased slightly with increases in product pressurizing pressure. For the PSA process, high purity of nitrogen was not available when argon was present in the feed mixture. High purity of nitrogen over 99% was observed by mode 4 when the feed mixture was free of argon, while the purity decreased to 98% with presence of argon in the feed mixture. Also, the same trend was detected by mode 3, where the purity decreased from 98% to 92% when argon was considered in the feed mixture. Only oxygen is adsorbed by CMS from the feed mixture (O<sub>2</sub>: 21%, N<sub>2</sub>: 78%, Ar: 1%). For different PSA modes, the equalization step in mode 3, and the equalization step with purging step under vacuum pressure in mode 4 are useful to increase the nitrogen purity to 99% in comparison with other modes (mode 1 and mode 2) where the nitrogen purity was about 90%. The best arrangement of all modes from higher to lower nitrogen purity is as follows: mode 4, mode 3, mode 2, and mode 1. For operation parameters, the purities of argon and nitrogen in the product stream increased with increases of adsorption pressure due to increases in adsorption capacity of CMS sieve to adsorb more oxygen. In all modes, the purity of nitrogen increased a few percent between adsorption times of 50 – 100 s. Also, the purity of nitrogen decreased about 4% with increases of purge flow rate from 1 to 6 liter/min, and optimum purge flow rate was between 1 and 2 liter/min.

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