Article

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Abstract: To enhance the oxygen guarantee capacity in high altitude areas and address the challenges of traditional pressure swing adsorption oxygen generation fixed equipment with large volume and multiple device modules, a novel single-reversible-pump single-bed vacuum pressure swing adsorption (VPSA) oxygen generation process was proposed and simulated. This study investigated the effects of purge on oxygen productivity, purity, recovery, and energy consumption, determining that the optimum ratio of total oxygen in the purge gas to the total oxygen in the feed gas (P/F) was 0.176. A set of principle prototypes was developed and validated in plains. The process performance was then simulated and studied at altitudes of 3000 m, 4000 m, and 5000 m. Finally, the optimization was carried out by adjusting the product flow rate and feed flow rate, revealing that the best performance can be achieved when the oxygen purity exceeded 90% with lower energy consumption or larger productivity than the optimization goal. This study serves as a valuable reference for the optimization of the VPSA oxygen generation process in a plateau environment.

Keywords: numerical simulation; plateau oxygen generation; vacuum pressure swing adsorption

1. Introduction

Oxygen supply is a vital measure for preventing and treating patients and injuries, especially in plateau areas with low oxygen content in the air, where oxygen deficiency can be life-threatening. The timely provision of oxygen is a critical measure to reduce the injury and death rate and improve life-saving capabilities. Hyperbaric oxygen therapy is a crucial treatment for acute traumatic brain injury, significantly improving physiological indicators and prognosis [1]. The demand for oxygen in the plateau region is high, but the transportation cost of oxygen is expensive, and the capacity is insufficient [2]. Among the commonly used oxygen generation methods, pressure swing adsorption (PSA) can continuously produce oxygen on site. It was first proposed by Skarstrom [3] in 1960 for a two-absorption bed four-step process for air separation. Now it has evolved an ideal separation method with high automation, low cost, and on-site gas production capability [4]. Air was separated by the difference in the loading of O₂ and N₂ adsorbed in the zeolite, and oxygen with a purity of over 90% was enriched by cyclic pressure changes [5].

In addition to experiments, numerical simulation was a vital alternative to studying the chemical processes. It enables the calculation of process performance under various conditions, and facilitates the exploration of data that were difficult to obtain through experimental methods [6]. Scholars have widely applied the simulation method to hydrogen enrichment [7,8], organic gas separation [9], and carbon dioxide capture [10,11]. Numerical simulation is already a well-established and effective research method to study...
the pressure swing adsorption process. In the high-altitude simulation, Tian et al. [12] studied the relationship between oxygen recovery and purity at increasing altitudes for plateau PSA oxygen production and found that an appropriate increase in flushing pore size was found to improve oxygen purity and that the relevant prolongation of adsorption time can increase oxygen concentration and recovery in highlands.

The high-pressure adsorption of the PSA process leads to high energy consumption. Energy saving was very valuable in highlands with limited oil delivery and fuel resupply [13]. For effective comparison, PSA, vacuum swing adsorption (VSA), and temperature swing adsorption (TSA) were modeled and optimized considering gas purity, energy consumption, and capital costs, and it was concluded that VSA was the superior process [14]. By comparing the process performance of the four-bed vacuum pressure swing adsorption (VPSA), TSA, and temperature vacuum swing adsorption (TVSA) processes in terms of feed volume, flushing rate, and vacuum level, it was found that VPSA had a clear advantage in terms of productivity and low energy consumption and was the most efficient process under the working conditions [15]. Marcoberrardino et al. [16] compared hydrogen production via PSA and VPSA processes through modeling and showed that VPSA has better recovery and purity. Luberti et al. [17] compared the VSA and PSA processes and improved the overall performance by integrating a two-stage VSA process design, with a pressure of 0.1–1 bar. It can be concluded that the vacuum pressure swing adsorption process is superior in terms of low energy consumption and improved process performance. Many scholars have also carried out simulation studies on the VPSA process. Kim J et al. [18] simulated that the VPSA method enhances the economic efficiency of recovering blast furnace gas. Punpee S et al. [19] used Aspen Adsorption to explore the optimal purge flow rate and vacuum pressure for VPSA. Makarem et al. [20] conducted an experimental and theoretical study of the VPSA oxygen generation process. The effects of adsorption time and purge pressure on oxygen recovery and purity were explored.

However, air compressors, cold dryers, air buffer tanks, and other pre-stage equipment were required in multi-bed processes [21]. Acklet [22] reviewed the small medical oxygen concentrator (MOC) air separation technology for oxygen production and described in detail the dual-bed VPSA oxygen production process, but the process described used two modules, an air compressor and a vacuum pump, for pressure conversion. Chicano J et al. [23] compared the 12-bed and 4-bed VPSA processes and showed that 4-bed VPSA could achieve the same purity goals as the 12-bed with lower recovery. Budner et al. [24] studied two-bed VPSA oxygen generation, producing oxygen with a purity of 90–94% O₂ (v/v). Mahdi A et al. [25] used Matlab to simulate four different configurations of the single-bed oxygen generation process to obtain a more economical and efficient design with 90% oxygen production concentration. Chinhd [26] simulated and experimented with single-bed nitrogen production, explored the partial pressure variation and optimized the process model. Their results illustrated that the reduction in the number of beds still ensures purity. Multi-bed process system composition and structure were complex and challenging to integrate; furthermore, the large size and difficulties in transport and maintenance reduced the environmental adaptability and mobility. The single-bed single-pump VPSA allowed for high integration while maintaining oxygen purity. As a result, the VPSA process offered outstanding advantages for oxygen production in high altitude conditions.

This study aimed at poor mobility and difficulties in the emergency rescue of traditional multi-bed VPSA equipment. In order to solve these issues, a novel single adsorption bed VPSA oxygen generation process based on a reversible pump was designed, utilizing the LiLSX molecular sieve as the adsorbent material. The adsorption isotherms were measured and a mathematical model was developed. The effects of the necessity of purging, forward purging, and backward purging on oxygen productivity, purity, recovery, and energy consumption per unit of oxygen were investigated. By exploring the optimum ratio of purge oxygen volume to total feed oxygen volume (P/F), an optimum process was established. A principal prototype consisting only of a single reversible pump, control module, single adsorption bed, purging module and buffer tank was built and verified.
Additionally, this study explored the effect patterns of altitude on the performance of oxygen generation. The process was optimized under altitude by adjusting the product flow rate and feed flow rate. Eventually, this process achieved oxygen generation equipment of medium-sized with lower energy consumption, which can adapt to different external environmental changes, with adjustable and controllable oxygen generation capacity.

2. Process and Mathematical Model for the VPSA System

2.1. Process of Single-Bed VPSA System

In this work, the single adsorption bed VPSA process is used to generate oxygen and the schematic diagram of the VPSA process is shown in Figure 1. Air was fed into the adsorption bed using a reversible Roots pump, with an adsorption pressure of approximately 1.7 bar. During vacuum operation, the Roots pump was reversed to reduce the pressure to around 0.5 bar. The adsorbent is the LiLSX-based adsorbent OX-19 produced by CECA (Paris, France). LiLSX zeolite has a high nitrogen–oxygen separation factor. The VPSA process consists of six steps operated in a cyclic model: Adsorption 1 (AD1), Adsorption 2 (AD2), Blowdown (BD), Vacuum (VU), Purge (PUR), and the final Pressurization (PR). Each cycle takes approximately 30–40 s to complete. Detailed descriptions of each step are provided below:

(I) Adsorption 1 (AD1): The pump operates in forward direction to introduce air into the adsorption bed. Due to the strong adsorptive capacity, N\textsubscript{2} is retained within the zeolite while the weakly adsorbed component O\textsubscript{2} is enriched and collected as the product gas through valve VP1.

(II) Adsorption 2 (AD2): The continuous operation of the pump allows oxygen-rich air to enter the purge buffer tank via valve VPU.

(III) Blowdown (BD): After the completion of the adsorption steps, the N\textsubscript{2} is expelled, the pump is switched reversely, and the high pressure can be released to atmospheric pressure. The adsorbent is initially desorbed.

(IV) Vacuum (VU): The pump operates in the reverse mode to lower bed pressure to approximately 0.5 bar for the further regeneration of the absorbent.

(V) Purge (PUR): The pump continues operating and the valve VPU is opened to allow the oxygen-enriched air to flow into the adsorption bed, further improving the desorption effect.

(VI) Pressurization (PR): The Roots pump changes the direction to positive. The initial pressurization of the bed is completed from the vacuum to atmospheric pressure.

Figure 1. Process schematic diagram of VPSA.
2.2. Mathematical Model

VPSA is a cyclic dynamic process with a strong inter-coupling of process parameters and complex mathematical models. The simulation design of the VPSA process using Aspen Adsorption software (v12) could save labor and material resources and allow an in-depth exploration of process details. Before simulation, the numerical model should be simplified appropriately and the assumptions are described below:

(a) The gas followed the ideal gas law.
(b) Adoption of a one-dimensional adsorption bed mathematical model.
(c) The pressure drop along the bed satisfied the Ergun equation.
(d) The mass transfer rate confirmed the linear driving force (LDF) model.
(e) The Extended Langmuir 2 equation was used to describe the adsorption behavior of the gas.
(f) A uniform distribution of adsorbent in the adsorbent bed and a uniform adsorbent bed void fraction.

Partial differential equations were utilized to describe the mass, momentum, and adsorption equilibrium of the bed. The gas–solid mass transfer model includes an axial diffusion mass transfer term, a convective mass transfer term, an accumulation term in the bed and adsorbent particles, and an adsorbent adsorption accumulation term. The mass balance equation for a component of the gas mixture during adsorption is expressed as:

\[-\varepsilon_i D_{ax,i} \frac{\partial^2 c_i}{\partial z^2} + \frac{\partial (v_g c_i)}{\partial z} + \left(\varepsilon_i + (1 - \varepsilon_i) \varepsilon_p \right) \frac{\partial c_i}{\partial t} + \rho_s (1 - \varepsilon_i) \frac{\partial q_i}{\partial t} = 0\]  \hspace{1cm} (1)

The axial dispersion coefficient of component \(i\), \(D_{ax,i}\), can be calculated according to Equation (2), where \(D_{m,i}\) is molecular diffusivity of component \(i\), \(v_g\) is gas velocity, \(r_p\) is particle radius, \(\varepsilon_i\) is interparticle voidage, and \(\varepsilon_p\) is intraparticle voidage.

\[D_{ax,i} = 0.73 D_{m,i} + \frac{v_g r_p}{\varepsilon_i \left(1 + 9.49 \varepsilon_i D_{m,i} \frac{v_g r_p}{v_g v_g}\right)}\]  \hspace{1cm} (2)

The momentum transfer model followed the Ergun equation as Equation (3), where \(\mu\) is dynamic viscosity, \(\rho_g\) is Gas density, \(\psi\) is sphericity.

\[-\frac{\partial P}{\partial z} = \frac{150 \mu (1 - \varepsilon_i)^2}{\varepsilon_i (2 r_p \psi)^2} v_g + 1.75 M \frac{(1 - \varepsilon_i) \rho_g}{2 r_p \psi \varepsilon_i} |v_g| |v_g|\]  \hspace{1cm} (3)

The Extended Langmuir 2 model was used for isothermal adsorption, as expressed in Equation (4). The model has a high predictive stability for the competitive adsorption of multi-component ideal gases, which was more in line with the reality. \(q_i^*\) is the amount of component \(i\) on the solid adsorbent in equilibrium conditions. \(IP_{1-4}\) are parameters related to adsorption amount.

\[q_i^* = \frac{IP_{k,i} P_{i,j}^{\beta_i} T_i}{1 + \sum_i \left( IP_{k,i} P_{i,j}^{\beta_i} T_i P_i \right)}\]  \hspace{1cm} (4)

The adsorption kinetics is described using the linear driving force (LDF) model, which offers a straightforward and computationally efficient mass transfer model as depicted in Equation (5), where \(q_i\) is the amount of component \(i\) on the solid adsorbent.

\[\frac{\partial q_i}{\partial t} = k_{LDF,i} (q_i^* - q_i)\]  \hspace{1cm} (5)
The adsorbent parameter is one of the most important parameters in the mathematical modeling. The static adsorption of N\textsubscript{2} and O\textsubscript{2} on LiLSX at different temperatures was measured and can be found in the Supplementary Materials. Based on the adsorption isotherm measurements and Equation (4), the parameters were fitted and other adsorbent bed parameters used in the simulation are shown in Table 1. Due to the proximity of argon and oxygen adsorption, the data for argon adsorption are the same as those for oxygen. The multi-component breakthrough experiments were carried out on a fixed bed; further details are given in the Supplementary Materials.

### Table 1. Parameters of adsorbent and adsorption bed.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>(H_b)</td>
<td>0.6</td>
<td>m</td>
</tr>
<tr>
<td>(D_b)</td>
<td>0.5</td>
<td>m</td>
</tr>
<tr>
<td>(\epsilon_i)</td>
<td>0.4</td>
<td>/</td>
</tr>
<tr>
<td>(\epsilon_p)</td>
<td>0.39</td>
<td>/</td>
</tr>
<tr>
<td>(p_b)</td>
<td>634.0</td>
<td>kg·m(^{-3})</td>
</tr>
<tr>
<td>(r_p)</td>
<td>8 \times 10(^{-4})</td>
<td>m</td>
</tr>
<tr>
<td>(D_{m, \text{Ar}})</td>
<td>4.137 \times 10(^{-5})</td>
<td>m(^2)·s(^{-1})</td>
</tr>
<tr>
<td>(D_{m, \text{N}_2})</td>
<td>2.491 \times 10(^{-5})</td>
<td>m(^2)·s(^{-1})</td>
</tr>
<tr>
<td>(D_{m, \text{O}_2})</td>
<td>4.137 \times 10(^{-5})</td>
<td>m(^2)·s(^{-1})</td>
</tr>
<tr>
<td>(I_{P1, \text{Ar}})</td>
<td>6.025 \times 10(^{-4})</td>
<td>mol·kg(^{-1})·bar(^{-1})</td>
</tr>
<tr>
<td>(I_{P1, \text{N}_2})</td>
<td>2.756 \times 10(^{-4})</td>
<td>mol·kg(^{-1})·bar(^{-1})</td>
</tr>
<tr>
<td>(I_{P1, \text{O}_2})</td>
<td>6.025 \times 10(^{-4})</td>
<td>mol·kg(^{-1})·bar(^{-1})</td>
</tr>
<tr>
<td>(I_{P2, \text{Ar}})</td>
<td>1593.0</td>
<td>K</td>
</tr>
<tr>
<td>(I_{P2, \text{N}_2})</td>
<td>2494.0</td>
<td>K</td>
</tr>
<tr>
<td>(I_{P2, \text{O}_2})</td>
<td>1593.0</td>
<td>K</td>
</tr>
<tr>
<td>(I_{P3, \text{Ar}})</td>
<td>1.487 \times 10(^{-4})</td>
<td>bar(^{-1})</td>
</tr>
<tr>
<td>(I_{P3, \text{N}_2})</td>
<td>1.391 \times 10(^{-4})</td>
<td>bar(^{-1})</td>
</tr>
<tr>
<td>(I_{P3, \text{O}_2})</td>
<td>1.487 \times 10(^{-4})</td>
<td>bar(^{-1})</td>
</tr>
<tr>
<td>(I_{P4, \text{Ar}})</td>
<td>1503.0</td>
<td>K</td>
</tr>
<tr>
<td>(I_{P4, \text{N}_2})</td>
<td>2449.0</td>
<td>K</td>
</tr>
<tr>
<td>(I_{P4, \text{O}_2})</td>
<td>1503.0</td>
<td>K</td>
</tr>
</tbody>
</table>

#### 2.3. Simulation Process and Strategy

The schematic diagram of sing-bed VPSA in simulation is illustrated in Figure 2. It should be noted that there was no reversible pump module in the software. Therefore, two modules of a pre-pump and a post-vacuum pump were utilized to simulate the reversible Roots pump. The energy consumption was calculated as the combined sum of these two pumps. To explore the purging factor, the circled portion of Figure 2 was excluded from the process without purging, resulting in a four-step process excluding the AD2 and PUR steps. As shown in Figure 2, PUMP is the inlet blower, and VF represents the valve. Bed is the adsorption bed; TD1 and TD2 are the dead volumes, \(\text{O}_2\) Tank is the product gas buffer tank, VP1 is the buffer tank inlet valve, and VP2 functions as the product outflow valve which remains open throughout cycle with its opening controlled using \(C_v\) (valve opening coefficient) set at 0.11 mol·s\(^{-1}\)·bar\(^{-1}\). VE is the equalization valve, and its \(C_v\) is 120 mol·s\(^{-1}\)·bar\(^{-1}\); WE is the equalization module; the pressure is equalized with the atmosphere through it in BD and PR steps. VPump is the vacuum pump and the \(C_v\) of valve VPU is 1.3 mol·s\(^{-1}\)·bar\(^{-1}\). The Cycle Organizer indicates the cycle controller operating based on parameters listed in Table 2. For valves within this simulation model, value “0” indicates closed status; value “1” indicates open status; and value “2” implies that the valve opening degree is controlled using \(C_v\).
The upwind differential scheme I (UDS1) method is used to discretize partial differential equations (PDEs). The axial spatial domain of the adsorption bed is discretized into 100 nodes. PDEs are converted into a series of differential-algebraic equations (DAEs). The MA48 solver and the Mixed Newton method are used to solve systems of linear and nonlinear equations. A cyclic steady state is considered to be reached when the difference between the cyclic variables of the two cycles is less than $10^{-5}$.

2.4. Data Analyses

During the VPSA process, five indicators would be analyzed and compared with the following simulation results under different conditions. $\text{Purity}_{O_2}$ is the purity at the outlet of the oxygen buffer tank, which is determined by Equation (6):

$$\text{Purity}_{O_2} = \frac{\int_{0}^{t_{\text{cycle}}} u_{\text{pro}} y_{\text{Pro,O}_2} \, dt}{\int_{0}^{t_{\text{cycle}}} u_{\text{pro}} y_{\text{Pro},i} \, dt} \times 100\%$$

where $t_{\text{cycle}}$ is the time of one cycle, $u_{\text{pro}}$ is the superficial velocity of product gas, $y_{\text{Pro,O}_2}$ is oxygen purity of product gas, and $y_{\text{Pro},i}$ is the purity of component $i$ of product gas.

The Recovery$_{O_2}$ is an important indicator to assess the performance of the process, which follows Equation (7):

$$\text{Recovery}_{O_2} = \frac{\int_{0}^{t_{\text{cycle}}} u_{\text{pro}} y_{\text{Pro,O}_2} \, dt}{\int_{0}^{t_{\text{cycle}}} u_{\text{pro}} y_{\text{Pro},i} \, dt} \times 100\%$$
Recovery_{O_2} = \frac{\int_0^{t_{cycle}} u_{Pro} y_{Pro,O_2} \, dt}{\int_0^{t_{cycle}} u_{Feed} y_{Feed,O_2} \, dt + \int_0^{t_{cycle}} u_{WE_Rev} y_{WE_Rev,O_2} \, dt} \times 100\% \quad (7)

where \( u_{feed} \) is the superficial velocity of feed, \( y_{Pro,O_2} \) is the oxygen purity of feed, \( u_{WE_Rev} \) is the superficial velocity of WE reverse and \( y_{WE_Rev,O_2} \) is the oxygen purity of WE reverse.

As the cycle reaches a steady state, each cycle is consistent in terms of the materials fed into and out of the cycle. Therefore, Productivity_{O_2} is calculated from a single cycle as Equation (8):

Productivity_{O_2} = 3600 \int_0^{t_{cycle}} u_{Pro} y_{Pro} \, dt \quad (8)

This study evaluated the energy consumption. The pump consumed the highest energy in this process, and the energy consumption varied greatly under different altitude conditions. As a consequence, only the energy consumption of the pump is calculated while neglecting the energy loss of the control module and measurement module. The formula for calculating energy consumption is shown in Equation (9):

Energy Consumption = \frac{\int_0^{t_{cycle}} \text{Power}_{Pump} \, dt}{3600} + \frac{\int_0^{t_{cycle}} \text{Power}_{VPump} \, dt}{3600 \int_0^{t_{cycle}} u_{Pro} y_{Pro} \, dt} \quad (9)

where \( \text{Power}_{Pump} \) is the energy that the pump uses and \( \text{Power}_{VPump} \) is the energy that the VPump uses.

The ratio of total oxygen in the purge gas to the total oxygen in the feed gas (\( P/F \)) is calculated using the following Equation (10):

\[ P/F = \frac{\int_0^{t_{cycle}} n_{Pur} y_{Pur,O_2} \, dt}{\int_0^{t_{cycle}} n_{Feed,O_2} \, dt + \int_0^{t_{cycle}} n_{WE_for,O_2} \, dt} \quad (10) \]

where \( n_{pur} \) is the amount of substance in the purge step, \( n_{WE_for,O_2} \) is the amount of substance in WE forward, \( n_{Feed,O_2} \) is the amount of substance in feed, and \( y_{Pur,O_2} \) is the \( O_2 \) purity of purge gas.

3. Process and Parameter Optimization

3.1. Effect of Purging on VPSA Performances

The process performance of VPSA is affected by a variety of conditions. In this work, simulations were conducted under different process conditions to investigate the effects of purging and the direction of the purge on the process performance. Table 3 shows the simulation results of purging. Three cases of no-purge (No-PUR), backward-purge (B-PUR), and forward-purge (F-PUR) were set for comparison. It should be noted that the No-PUR case corresponds to a four-step cycle operation, ignoring the AD2 and PUR steps. As shown in Table 3, the oxygen purity in the backward purging process is 92.22%. The highest recovery rate is observed at 17.39%, with a productivity of 3.68 m^3·h^{-1}, energy consumption of 1.58 MJ·m^{-3} and the P/F of 0.18. Only the B-PUR process meets the medical standard requirement for oxygen concentration (>90%) [28], indicating that backward purge flow effectively enhances oxygen purification. The reasons should be that in the No-PUR cycle, due to the lack of purging, the \( N_2 \) solid-phase concentration remains high, leading to incomplete adsorbent desorption. In the B-PUR process, the vacuum pump purges a high oxygen concentration from the top to the bottom of the adsorption bed, rapidly reducing the solid phase concentration of \( N_2 \). The desorption of the adsorbent is promoted. On the contrary, in the F-PUR cycle, purged gas enters from the bottom but gets pumped out directly without regeneration as the vacuum pump runs continuously, resulting in a longer mass transfer zone but lower oxygen purity. In Equation (8), all the gases at the
outflow end are qualified. In reality, however, in F-PUR processes, the oxygen purity does not reach 90%, which leads to an inflated production. Therefore, the optimal condition is backward purging, which is consistent with the conclusions of J C Santos [29]. Subsequent investigations are carried out based on this optimized condition.

Table 3. Simulation results of purging.

<table>
<thead>
<tr>
<th></th>
<th>Recovery %</th>
<th>Purity %</th>
<th>Productivity m³·h⁻¹</th>
<th>Energy Consumption MJ·m⁻³</th>
<th>P/F</th>
</tr>
</thead>
<tbody>
<tr>
<td>No-PUR</td>
<td>13.32</td>
<td>81.33</td>
<td>3.35</td>
<td>1.58</td>
<td>/</td>
</tr>
<tr>
<td>B-PUR</td>
<td>17.39</td>
<td>92.22</td>
<td>3.68</td>
<td>1.58</td>
<td>0.18</td>
</tr>
<tr>
<td>F-PUR</td>
<td>14.82</td>
<td>74.18</td>
<td>3.98</td>
<td>1.51</td>
<td>0.15</td>
</tr>
</tbody>
</table>

3.2. Effect of P/F on VPSA Performances

The effect of P/F on \( \text{O}_2 \) purity, recovery, productivity, and energy consumption is shown in Figure 3, with the P/F corresponding to the AD2 duration. As the AD2 duration increases, the volume of purge gas expands and oxygen purity rises from 89.76% to 92.34%. \( \text{O}_2 \) Recovery increases from 15.44% to 19.39%. Figure 3b shows that \( \text{O}_2 \) Productivity escalates from 3.31 m³·h⁻¹ to 4.17 m³·h⁻¹, and energy consumption declines from 1.60 MJ·m⁻³ to 1.49 MJ·m⁻³. The reason for this can be seen in Table 4. It demonstrates the P/F, the VU and AD2 pressure ratios for different AD2 times. Table 4 reveals that the P/F increased by nearly double at 2 s compared to 1 s, and the purge volume increased significantly, leading to a more thorough desorption and a significant increase in purity and energy consumption. At 3–5 s AD2 time, the purging gas volume increases less. However, due to the continuous operation of the pump in AD2, \( P_{\text{AD2}} \) increases to the point of exceeding the operating pressure setting of the reversible pump (1.7 bar). Therefore, considering pump loading factors, an appropriate increase in P/F is favorable for the process enhancement of VPSA. This is in accordance with Liu’s conclusions [30] and is much lower than their P/F value of 0.51.

![Figure 3. Cont.](image-url)
The pressure change in the adsorption bed during a cycle is shown in Figure 3. Effects of purge time on (a) purity, recovery and (b) productivity and energy consumption in the plain area.

![Graph showing productivity and energy consumption over AD2 time](image)

**Figure 3.** Effects of purge time on (a) purity, recovery and (b) productivity and energy consumption in the plain area.

<table>
<thead>
<tr>
<th>AD2 Time</th>
<th>P/F</th>
<th>PVU/PAD2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 s</td>
<td>0.081</td>
<td>0.51/1.66</td>
</tr>
<tr>
<td>2 s</td>
<td>0.153</td>
<td>0.51/1.65</td>
</tr>
<tr>
<td>3 s</td>
<td>0.176</td>
<td>0.52/1.69</td>
</tr>
<tr>
<td>4 s</td>
<td>0.190</td>
<td>0.52/1.74</td>
</tr>
<tr>
<td>5 s</td>
<td>0.198</td>
<td>0.53/1.79</td>
</tr>
</tbody>
</table>

**Table 4.** P/F and PVU/PAD2 at different times for AD2.

3.3. **Solid Phase Concentration and Pressure Distribution in the Adsorption Bed**

The solid phase concentration distribution in the adsorption bed is the most visually representative data reflecting the adsorption situation, and the method of the numerical calculation simulation can quickly obtain the solid phase concentration distribution. Figure 4a,b show the solid phase concentration distribution of N₂ and O₂ in the bed at the end of each step. As the adsorption step proceeds, the adsorption front moves forward. It can be seen from the figure that the adsorption front is located in the upper middle of the bed at the end of the AD step. Additionally, the solid phase concentration of O₂ shows a gradually increasing trend with the increase in axial distance. This is because after the AD step is completed, N₂ is adsorbed in large amounts in the bed, and the O₂ gradually increases in the latter part of the bed, and consequently, the solid phase concentration also rises. After the BD, VU, and PUR steps, the pressure decreases. N₂ is desorbed, and the solid phase concentration is minimized. Since purging involves using O₂, the O₂ solid phase concentration distribution picks up after purging. The last step of PR is pressure boosting for raw gas, which results in a rise in both N₂ and O₂ concentrations.

The pressure change in the adsorption bed during a cycle is shown in Figure 5. During AD1 lasting for 10 s, pressure increases from atmospheric to 1.65 bar. As AD2 proceeds for 3 s, the pressure fluctuates slightly due to the valve VPU opening connected to the purge buffer tank. The BD step is then performed for 3 s, and the pressure rapidly decreases to 1.013 bar. Then, as VU is performed, the pressure is gradually reduced to 0.5 bar. The PUR step is performed when the VPU is opened for purging, which results in pressure back-up fluctuation. At the end of the cycle is the PR step, where the pressure rapidly rises to 1.013 bar.
Figure 4. Axial distribution of N\textsubscript{2} (a) and O\textsubscript{2} (b) on solid phase at the end of each step.

Figure 5. Pressure distribution diagram of VPSA adsorption bed.
4. Simulation Verification

Simulated breakthrough curves were utilized to validate the accuracy of the critical parameters of the adsorption bed. Detailed information can be found in the Supplementary Materials. In this work, a prototype was constructed for calculating and optimizing the oxygen generation demand, as shown in Figure 6. Air is fed using a reversible Roots pump (SSR-80H, Shandong Zhanghuang Machinery Industry Co., Zhangqiu, China) to the adsorption bed at a temperature of 298 K. The pressure transition during the process is achieved by controlling the direction of the operation of the Roots pump, which can run both forward and backward. The Roots pump is controlled using a Programmable Logic Controller (PLC, Horner-He-Exl1e2) system via a variable frequency converter. Prior to usage, vacuum regeneration is performed on the adsorbents. Following nitrogen adsorption, enriched oxygen flows into an oxygen buffer tank through a non-return valve and serves as product gas.

![Figure 6. Schematic diagram of VPSA oxygen generation.](image)

Table 5 compares the six-step cycle simulation results with the VPSA process experimental results. Performance indicators such as VU/AD pressure, purity, and productivity were considered in this comparison analysis. The conditions were all as follows: the ambient temperature was 298 K, the altitude was at sea level, and the environmental pressure was of 1.013 bar. The AD2 time was set to 3 s, and the direction of purging was backflush. The experiment was repeated three times to reduce the operating and random errors. The values showed excellent agreement between the experiment and simulation. Excellent agreement between experimental data and simulation results was observed under different conditions, confirming the accurate establishment of our simulation model for predicting experimental outcomes. By comparing with Lu et al. [31], the unit energy consumption of the six-bed VPSA process is 0.504 k·Wh·m⁻³, while the unit energy consumption of this single-bed VPSA prototype is 0.305 k·Wh·m⁻³, which achieves low energy consumption.

<table>
<thead>
<tr>
<th>VU/AD Pressure (bar)</th>
<th>Purity (%)</th>
<th>Productivity (m³·h⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Exp.</td>
<td>Sim.</td>
</tr>
<tr>
<td>0.52/1.69</td>
<td>92.1</td>
<td></td>
</tr>
<tr>
<td>0.51/1.67</td>
<td>93.2</td>
<td>0.51/1.69</td>
</tr>
<tr>
<td>0.48/1.68</td>
<td>91.5</td>
<td></td>
</tr>
</tbody>
</table>

Table 5. Comparison between experimental and simulation results.
5. Plateau Process Optimization

5.1. Effect of Altitude on VPSA Performances

The impact of altitude on oxygen purity, recovery, productivity, and energy consumption is shown in Figure 7. The investigated plateau conditions include the altitudes of 3000 m, 4000 m and 5000 m, corresponding to external pressures of 0.701 bar, 0.617 bar, and 0.54 bar. The temperature is maintained at 298 K and under 3 s of purging conditions. As shown in Figure 7a, the oxygen purity exhibits slight fluctuations above the threshold of 92% as the altitude increases. The recovery shows a decreasing trend from 15.64% to 14.66%, and the reason for this is that the oxygen becomes thinner as the altitude increases. As shown in Figure 7b, the oxygen production decreases from 2.31 m$^3$·h$^{-1}$ to 1.68 m$^3$·h$^{-1}$ with increasing altitude. The energy consumption rises from 1.65 MJ·m$^{-3}$ to 1.70 MJ·m$^{-3}$. The thinning of the air leads to a reduced oxygen content, less air entering the adsorption bed, and a consequent reduction in productivity. As the altitude increases in the plateau, it becomes more challenging for pumps to perform, and the energy consumption rises gradually.

![Figure 7](image_url)

**Figure 7.** Effect of altitude on (a) purity and recovery and (b) productivity and energy consumption.

Figure 8 shows the effect of altitude on the pressure range, i.e., the difference between the maximum adsorption pressure and minimum vacuum pressure during a single cycle. It can be seen that with the increase in altitude, the pressure range gradually diminishes. For the adsorbent, combined with its adsorption isothermal equation, it can be seen that its equilibrium adsorption capacity decreases with the decrease in pressure range, the adsorption capacity of N$\textsubscript{2}$ decreases, and the decrease in adsorption performance also leads to the decrease in productivity. At the same time, due to the low external environment in...
the high altitude area, the vacuum degree is increased, which reduces the negative impact caused by the reduction in the pressure range to a certain extent.

![Pressure vs Altitude](image)

**Figure 8.** Effect of altitude on the pressure range.

5.2. Effect of Product Flowrate on VPSA Performance

For medical oxygen production, it is important to have a wide range of product flow rate adjustments, and this chapter explores the effect of oxygen product flow rate on process performance at 3000 m, 4000 m, and 5000 m. This is achieved by adjusting the Cv of VP2. The results are shown in Figure 9. With the increase in the valve opening, the oxygen productivity increases, but the fluctuation of the oxygen flow rate becomes larger, and the oxygen purity decreases. At the increase to 1.7 mol·s⁻¹·MPa⁻¹, the concentrations all decrease to less than 90%. The recovery shows an increasing trend with increasing the product flow rate; it augments the utilization of the adsorbent bed and lengthens the mass transfer zone. When only the Cv is adjusted, the unit energy consumption decreases due to increased oxygen productivity. It can be seen that under the condition of the Cv maximum of 1.6 mol·s⁻¹·MPa⁻¹, the VPSA process can achieve the highest performance of 90% purity. The oxygen productivity of 3000 m is 3.25 m³·h⁻¹, the recovery is 21.64%, the energy consumption is 1.14 MJ·m⁻³; the oxygen productivity of 4000 m is 2.77 m³·h⁻¹, the recovery is 20.89%, and the energy consumption is 1.15 MJ·m⁻³. The productivity of 5000 m is 2.37 m³·h⁻¹, the recovery is 20.36% and the energy consumption is 1.17 MJ·m⁻³.

![O2 Purity and Recovery vs Cv](image)

**Figure 9.** Cont.
5.3. Effect of Feed Flowrate on VPSA Performance

In changing the value of the feed flow rate of the simulation model, it was observed that an increase in Cv led to a decrease in oxygen productivity. To ensure oxygen purity and meet production demands under different conditions, simulations were conducted with feed flow rates of 160 m³·h⁻¹, 180 m³·h⁻¹, 200 m³·h⁻¹, 220 m³·h⁻¹, 240 m³·h⁻¹, along with a Cv ranging from 1.2 mol·s⁻¹·MPa⁻¹ to 1.5 mol·s⁻¹·MPa⁻¹. With the increase in altitude at a constant feed flow rate, both the oxygen productivity and recovery gradually decrease while energy consumption per unit of oxygen increases. However, at the same altitude, the oxygen recovery and productivity increase with the increase in air intake, and the purity remains fluctuated above 90%. The changing trend of energy consumption per oxygen unit first decreases and then increases, as shown in Figure 10a–d. It shows the influence of different feed flow rates on energy consumption at altitudes of 3000 m to 5000 m under the conditions of valve opening from 1.2 mol·s⁻¹·MPa⁻¹ to 1.5 mol·s⁻¹·MPa⁻¹. It can be seen from the figure that there is the lowest energy consumption per unit of oxygen, and when the intake volume is 200 m³·h⁻¹, the energy consumption per unit of oxygen is the lowest under all working conditions. The reason can be obtained from Figure 11, which shows the trends in productivity and energy consumption with the increasing feed with the Cv of 1.4 mol·s⁻¹·MPa⁻¹ (the Cv of 1.4 mol·s⁻¹·MPa⁻¹ is shown here as an example for plotting). When the inlet volume increases, the pump continues to perform work, resulting in an increase in energy consumption and a corresponding rise in productivity. However, once the inlet volume exceeds 200 m³·h⁻¹, the energy consumption exhibits a more pronounced increase with a steeper curve. From Equation (9), it is known that the energy consumption is determined by both pump consumption and oxygen productivity within a single cycle. Consequently, there are optimal conditions that minimize energy consumption and guide the selection of process parameters for plateau environments. In combination with the difficulty of oil transportation in plateau areas, with low energy consumption as the optimization goal, the optimal feed flow rate of vacuum pressure swing adsorption oxygen generation in the single adsorption bed at a high altitude was 200 m³·h⁻¹. The energy consumption per unit of oxygen can reach 1.16 MJ·m⁻³ at 3000 m when the oxygen productivity is 4.03 m³·h⁻¹, the recovery rate is 23.43%, and the purity is 90.29%. At 4000 m, the minimum energy consumption is 1.18 MJ·m⁻³ with an oxygen productivity of 3.45 m³·h⁻¹, a recovery of 22.70%, and a purity of 90.33%. The lowest energy consumption per unit at 5000 m is 1.19 MJ·m⁻³. When taking oxygen productivity...
as the optimization target, the maximum oxygen productivity at 3000 m, 4000 m and 5000 m altitude can reach 4.93 m$^3$$\cdot$h$^{-1}$, 4.22 m$^3$$\cdot$h$^{-1}$ and 3.59 m$^3$$\cdot$h$^{-1}$, respectively. In particular, after the optimization, the performance evaluation indexes such as oxygen productivity are higher than those in the plain area, which is due to the maximum pressure load of the reversible pump of 1.7 bar. Figure 8 shows that the adsorption pressure in the high-altitude area was lower than in the plain area. This makes it possible to further increase the intake volume in the low-pressure area of the plateau to pressurize the adsorption bed without exceeding its critical pressure load.

![Graphs showing energy consumption and productivity at different altitudes](image)

**Figure 10.** Energy consumption at different altitudes with different feed flowrates at Cv of (a) 1.2 mol·s$^{-1}$·MPa$^{-1}$; (b) 1.3 mol·s$^{-1}$·MPa$^{-1}$; (c) 1.4 mol·s$^{-1}$·MPa$^{-1}$; (d) 1.5 mol·s$^{-1}$·MPa$^{-1}$.

![Graphs showing productivity and energy consumption at different altitudes](image)

**Figure 11.** Effects of feed on energy consumption and productivity at different altitudes with Cv of 1.4 mol·s$^{-1}$·MPa$^{-1}$.
6. Conclusions

In this study, the molecular sieve LiLSX was employed as the adsorbent, and air was taken as the feed gas to simulate the oxygen generation process in a single adsorption bed VPSA. The adsorption isotherms and other parameters were fitted. A mathematical model of the adsorption bed for this process was established. A prototype of a single reversible pump single-bed VPSA oxygen generation system was built and agreed with simulation results. Purge factors (No-PUR, B-PUR, F-PUR) were explored, revealing that a backward purge step was required to promote gas desorption from the zeolite to achieve high oxygen purity (above 90%) and the optimal P/F ratio was 0.176.

Altitudinal changes in the plateau (3000 m, 4000 m, and 5000 m) were also studied using simulation. The performance was significantly lower compared to that on the plains. The product and feed flow rates were further adjusted to obtain the maximum process performance. Finally, through the regulation of double conditions, the plateau performance reached or exceeded the plain oxygen generation level. This process holds a wide application prospect and a great potential for emergency rescue in the field area.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/pr12051015/s1, Figure S1: Adsorption isotherms for nitrogen and oxygen; Figure S2: (a) Adsorption amount of N\textsubscript{2} at different pressures and temperatures, (b) Adsorption amount of O\textsubscript{2} at different pressures and temperatures; Figure S3: Experimental and simulated breakthrough results; Figure S4: Breakthrough model in Aspen Adsorption; Table S1: Adsorption isotherm parameter fitting results; Table S2: Simulation results of different feed flow rates and Cv at 3000 m; Table S3: Simulation results of different feed flow rate and Cv at 4000 m; Table S4: Simulation results of different feed flow rate and Cv at 5000 m.

Author Contributions: Conceptualization, Y.Z. (Yanjun Zhang); simulation and optimization, Y.Z. (Yingying Zhang); validation, B.W. and H.S.; formal analysis, Y.Z. (Yingying Zhang), J.S. and Y.L.; writing—original draft preparation, Y.Z. (Yingying Zhang) and Y.L.; writing—review and editing, Y.Z. (Yanjun Zhang); project administration, Z.S., Y.Z. (Yanjun Zhang) and J.M.; funding acquisition, Y.Z. (Yanjun Zhang) and J.M. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflict of interest.

Nomenclature

The nomenclature involved in the text is as follows:

- $c_i$: gas phase concentration of component $i$, mol·m$^{-3}$
- $Cv$: valve opening coefficient, mol·s$^{-1}$·bar$^{-1}$
- $D_{ax,i}$: axial dispersion coefficient of component $i$, m$^2$·s$^{-1}$
- $D_{m,i}$: molecular diffusivity of component $i$, m$^2$·s$^{-1}$
- $H_b$: height of adsorbent layer, m
- $IP_1$: isotherm parameter, mol·kg$^{-1}$·bar$^{-1}$
- $IP_2$: isotherm parameter, K
- $IP_3$: isotherm parameter, bar$^{-1}$
- $IP_4$: isotherm parameter, K
- $k_{LDF,i}$: liner driving force constant of component $i$, s$^{-1}$
- $n_{Feed,O_2}$: amount of substance of $O_2$ in feed, mol
- $n_{WE_for,O_2}$: amount of substance of $O_2$ in WE forward, mol
- $n_{pur}$: amount of substance in the purge step, mol
- $P$: pressure, pa
- $P_i$: pressure of component $i$, pa
- $q_i$: amount of $i$ on the solid adsorbent, mol·kg$^{-1}$
- $q_i^*$: amount of $i$ on the solid adsorbent in equilibrium conditions, mol·kg$^{-1}$
- $R$: universal gas constant, (Pa·m$^3$)/(mol·K)
References


\[ R^2 \] adsorption model fitting correlation coefficients

\[ r_p \] particle radius, m

\[ T \] temperature, K

\[ t_{cycle} \] time of cycle, s

\[ u_{Feed} \] superficial velocity of feed, m\(^3\)s\(^{-1}\)

\[ u_{pro} \] superficial velocity of product gas, m\(^3\)s\(^{-1}\)

\[ u_{WE_Rev} \] superficial velocity of WE reverse, m\(^3\)s\(^{-1}\)

\[ v_g \] gas velocity, m/s

\[ y_{Feed, O2} \] O\(_2\) purity of feed

\[ y_{pro, i} \] Purity of component i of product gas

\[ y_{pro,O2} \] O\(_2\) purity of product gas

\[ y_{pur,O2} \] O\(_2\) purity of purge gas

\[ y_{WE_Rev,O2} \] O\(_2\) purity of WE reverse

\[ z \] axial distance, m

\[ \epsilon_i \] Interparticle voidage

\[ \epsilon_p \] Intraparticle voidage

\[ \mu \] Dynamic viscosity, kg m\(^{-1}\)s\(^{-3}\)

\[ \rho_b \] Bulk solid density of adsorbent, kg m\(^{-3}\)

\[ \rho_g \] Gas density, kg m\(^{-3}\)

\[ \rho_s \] adsorbent density, kg m\(^{-3}\)

\[ \psi \] Sphericity


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