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Pressure swing adsorption using flexible metal-organic framework for CO_2 capture from industrial sources

František Mikšík[a,*], Hiroshi Kajiro[b], Keisuke Ikeda[c], Yuya Takakura[c], Tomoyuki Yajima[c], Junpei Fujiki[a], Yoshiaki Kawajiri[a,c]

[a]*Research Centre for Net-Zero Carbon Society, Institute of Innovation for Future Society, Nagoya University, Nagoya 464-8603, Japan*
[b]*CCUS Technology Research Department, Japan Steel Corporation, Chiba 293-0011, Japan*
[c]*Department of Materials and Process Engineering, Graduate School of Engineering, Nagoya University, Nagoya 464-8603, Japan*

Abstract

Flexible metal-organic frameworks are a unique group of adsorption materials distinguished by high selectivity and typically S-shaped isotherm. The working principle is built around their capability of changing its structure depending on the adsorbate's relative pressure. However, due to the complexity of such characterization, their possible applications require rigorous testing. In this context, we introduce an ELM-11 adsorbent for CO_2 gas separation from industrial sources where the CO_2 concentration is in the range between 5 and 30%. This study presents experimental demonstration of laboratory-scale pressure swing adsorption (PSA), which is used to validate a mathematical model. Depending on the feed gas concentration of CO_2, flow rate and adsorption and desorption step times, we observed experimentally recovery up to 58.9 % with purity of the product CO_2 around 96.0 % at the feed gas pressure of about 0.9 MPa, which agrees well with the predictions given by the model. The power requirement is between 1.83 and 8.62 GJ/tCO_2 depending on the feed gas flow rate.
Keywords: Flexible MOF; Pressure Swing Adsorption, Metal Organic Framework;

1. Introduction

Metal-organic frameworks (MOF) has been gaining attention as effective adsorbents with adjustable adsorption characteristics. Specifically, applications requiring high selectivity for gas separation such as CO_2 capture can profit from the unique properties of MOF adsorbents [1]. However, MOF adsorbents are typically sensitive to preparation methods and conditioning, and for practical deployment an in-depth analysis of the adsorbents and targeted adsorption conditions is of paramount importance.

In this work, we report mathematical modeling and experimental validation of a pressure swing adsorption (PSA) process using ELM-11, a member of MOF materials with flexible structures. The model is based on the work of Fujiki et al. [2] where model parameters were estimated by a breakthrough analysis. Our model enables design and analysis of scaled-up systems, estimating recovery, purity and energy requirements. In addition, a bed size factor (BSF) as a measure of necessary adsorbent amount and energy consumption are evaluated.

2. Materials and laboratory-scale pressure swing adsorption system

ELM-11 is a MOF with a layered geometry that changes its shape in the presence of a sufficient pressure of an adsorbate [4] (Fig. 1). In this adsorbent, adsorption occurs with a structural change (gate-opening) at a certain pressure, called gate pressure. Due to this structural change, the crystal volume change, which does not allow typical palletization. For this problem, porous composite granules using a flexible substrate and binder were used instead [2]. Furthermore, structural change can be induced only by CO_2, but not by nitrogen, leading to high selectivity. The preparation of the raw pre-ELM-11 and conditioning was done by a conventional preparation method according to the literature, which can be found elsewhere [2][3].

Flexible MOF adsorbents with S-shaped adsorption isotherms offer the advantage of high-purity CO_2 product due to the high selectivity. However, the S-shaped isotherms also introduce challenges. Specifically, these adsorbents require a minimum pressure threshold (gate pressure) to activate adsorption. Consequently, any adsorbate below this pressure passes through the bed, so called "slipping off", leading to a loss of CO_2 and lower recovery. This undesirable operation should be avoided by choosing the operating conditions carefully, which can be guided by the mathematical model.

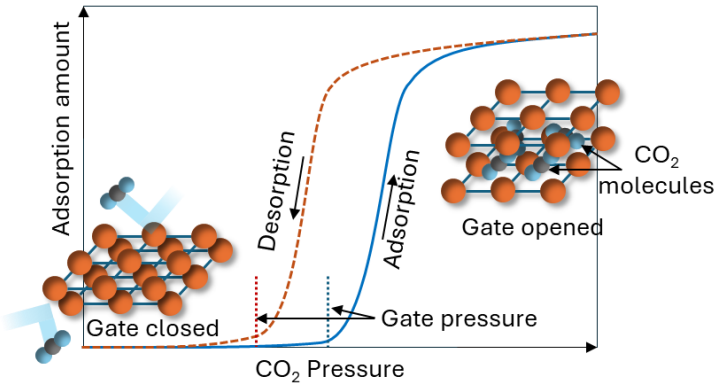

Fig.1: Illustration of isotherm hysteresis with the gate-opening/closing property of ELM-11

To experimentally validate the concept of an adsorption process using ELM-11, we performed a series of PSA tests. A laboratory-scale PSA unit packed with ELM-11 was used, and the collected data were used to validate the mathematical model of a single-column adsorber. A schematic of the experimental unit and profiles of concentration and temperature are shown in Fig.2 Several different operating conditions were tested with a variation in the feed gas pressure of around 0.9 MPa, flow rates of 500-2000 sccm, and temperatures of 25-30 ℃.

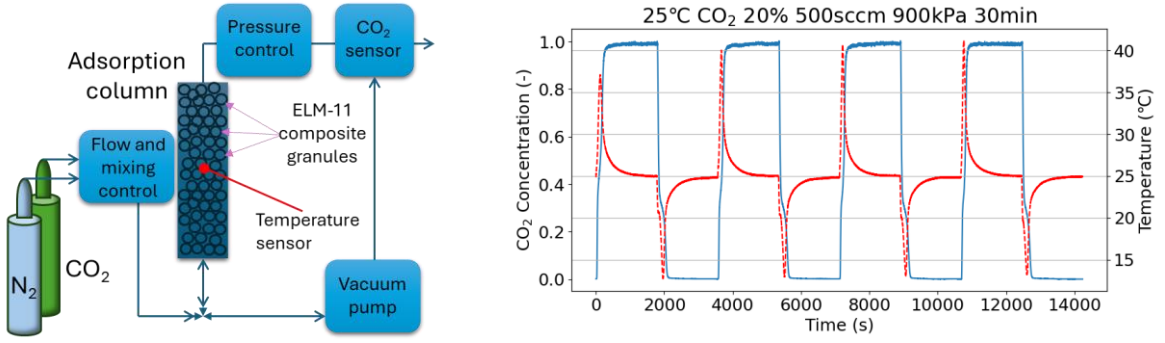

*Fig.2: **Left**-PSA experimental system schematics, **Right**-Cycles of adsorption and desorption (continuous line – CO_2 concentration, dashed line – adsorbent temperature in the middle)*

3. Results and discussion

In our experiments, the purity of the product CO_2 was consistently high, 95.5 % on average, which is slightly lower than the model's prediction, 99%. The slightly lower experimental value is given by the dead volume that was necessary to accommodate for higher flexibility in possible gas flow and configuration settings. The accuracy of the model can be observed in Fig.3 showing a close fit of the temperature measured in the PSA experiment. In the left subfigure in Fig.3 it can be seen that the predictions by the model capture the trend of experimental recovery well.

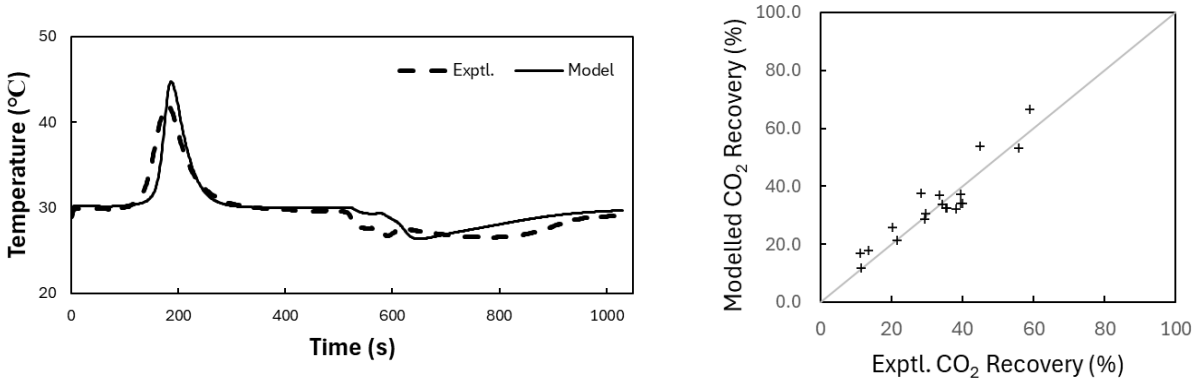

*Fig.3: **Left**- temperature profile comparison of the model and experimental result, **Right**-comparison of model predictions and experimental measurements on recovered CO_2 fraction*

Careful selection of operating parameters plays a key role in improving CO_2 recovery, which is also one of the primary objectives of the developed model. The recovery of CO_2 varies significantly across different operating conditions. Under the selected experimental conditions in the span 10 % to 30% of CO_2 in the feed gas, the recovery ranged from 11.4% to 58.9%. Notwithstanding, with optimized system design and operating conditions, the recovered CO_2 fraction is expected to exceed these values significantly. This variability underscores the critical importance of optimizing operating conditions to realize an effective CO_2 capture process, which can be achieved using the predictions given by the mathematical model, as demonstrated in Fig. 3.

In addition to purity and recovery, an important performance metric is the necessary amount of adsorbent. For this estimation, we use the beds size factor (BSF):

$$BSF\ \left[\frac{kg_{ads}}{TPDCO_2}\right] = \frac{m_{ads} \cdot t_{cycle}}{Mw_{CO_2} \cdot product} \times \frac{10^6}{24 \times 3600} \qquad (1)$$

where m_{ads} is the adsorbent weight, t_{cycle} is the cycle duration, Mw_{CO_2} is a molecular weight of CO_2, and the *product* is the molar amount of the recovered CO_2. It can be seen that the lower value of BSF means less amount of adsorbent to achieve the separation. BSF should be minimized by the optimization of the cycle by shortening the cycle time, and increasing the feed flow rate. The value of BSF in our experiment can be as low as 88.3 $kg_{ads}/TPDCO_2$ with the feed gas with 30% CO_2. Similarly, it is reasonable to expect improvement of BSF value with further optimized bed design and operating conditions.

Power consumption is also estimated, which consists of two main energy requirements, the compressor to increase the feed gas pressure to the operating value of 0.9 MPa and a vacuum pump necessary to bring the pressure in the column below gate-pressure for desorption. The estimated value is from 1.83 to 8.78 GJ/tCO_2 when the flow rate of the feed gas flow was between 500 sccm and 2000 sccm.

4. Conclusion

An experimental validation of a pressure swing adsorption (PSA) process using a flexible metal organic framework (MOF), ELM-11, was reported. The mathematical model we proposed previously agreed well with the experimental measurements at various conditions. It was also found that the CO_2 purity measured in the experiment was consistently high. Furthermore, productivity and energy consumption were found to be promising. The mathematical model validated in this study will serve as a powerful tool to optimize the design and operation of the PSA process, leading to significant improvements in key performance indicators introduced in this work.

Acknowledgment

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