Applied Thermal Engineering 128 (2018) 818–829

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng

Research Paper

Thermodynamic research of adsorbent materials on energy efficiency of vacuum-pressure swing adsorption cycle for CO_2 capture

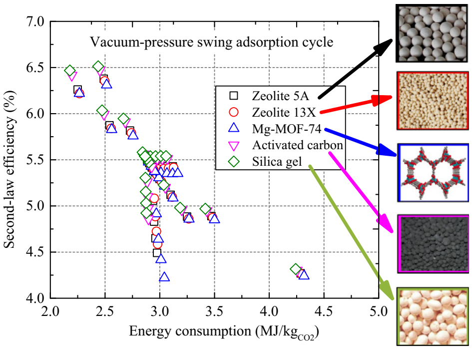
Ruikai Zhao[a], Shuai Deng[a,*], Shengping Wang[b], Li Zhao[a], Yue Zhang[a], Bowen Liu[a], Hailong Li[c], Zhixin Yu[d]

[a] *Key Laboratory of Efficient Utilization of Low and Medium Grade Energy (Tianjin University), Ministry of Education of China, Tianjin 300350, China*
[b] *Key Laboratory for Green Chemical Technology, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China*
[c] *School of Business, Society and Engineering, Mälardalen University, SE-72123 Västerås, Sweden*
[d] *Department of Petroleum Engineering, University of Stavanger, 4036 Stavanger, Norway*

HIGHLIGHTS

- Adsorbent effects on the energy-efficiency performance of VPSA are investigated.
- Mg-MOF-74, zeolite 13X, zeolite 5A, activated carbon and silica gel are compared.
- For the 5 adsorbent materials, the highest second-law efficiency is silica gel.
- Proportionality factor of working capacity is a key parameter for cycle design.
- The development of new adsorbents for Type III would be extremely urgent for VPSA.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 18 July 2017
Revised 30 August 2017
Accepted 15 September 2017
Available online 18 September 2017

Keywords:
VPSA
Second-law efficiency
Adsorbent materials
Carbon capture

ABSTRACT

This paper presents a comprehensive thermodynamic research on energy efficiency of vacuum-pressure swing adsorption (VPSA). The study examined the influence from four types of typical adsorbent materials on the energy efficiency of VPSA by cycle parameters. The selected adsorbent materials are activated carbons, zeolite 5A, zeolite 13X, silica gels, and metal-organic frameworks (MOFs). The study also analyzes the effects of separation temperature, adsorption pressure, desorption pressure, CO_2 concentration and percent of unused bed on the energy-efficiency of VPSA cycle. The examined performance parameters are CO_2 working capacity, proportionality factor, energy consumption and second-law efficiency. The results show that the energy consumption is approximately 2.0–4.5 MJ/kg and the second-law efficiencies are 4–7% for VPSA cycles using the five adsorbent materials. The effect of adsorbent materials on the energy efficiency mainly depends on the proportionality factor of CO_2 working capacity (β) of VPSA cycle, which is important to screen materials at the fixed cyclic boundary conditions and preliminary calculation of second-law efficiency for VPSA cycles. For existing adsorbent materials which are Type I commonly, the lower values of β would lead to the higher second-law efficiencies. The development of new adsorbents of Type III would be extremely urgent in near future.

1. Introduction

In the recent years, significant efforts have been invested in the field of materials and processes to capture CO_2 from anthropogenic

---

* Corresponding author.
E-mail address: sdeng@tju.edu.cn (S. Deng).

http://dx.doi.org/10.1016/j.applthermaleng.2017.09.074
1359-4311/

Nomenclature

Symbol

C_{CO2}	amount of CO_2 capture per cycle (mol)
EC	energy consumption (kJ/mol)
Eff_{2nd}	second-law efficiency (%)
k	polytropic parameter
P	pressure (bar)
q	amount of CO_2 adsorption (mol/kg)
R	universal gas constant (8.314 J/mol K)
Re_{CO2}	CO_2 recovery rate (%)
T	temperature (K)
V	volume of adsorber (m^3)
W	work consumption (kJ)
WC	working capacity (mol/kg)
y_{CO2}	CO_2 concentration (vol%)

Subscripts

ac	actual
ad	adsorption
atm	atmosphere
com	air compressor
dep	depressurization
eva	evacuation
min	minimum
pre	pressurization
vac	vacuum pump

Greek letters

β	proportionality factor of CO_2 working capacity
θ	specific value of differential pressure
ε	porosity
η_{unused}	percentage of unused bed (%)

sources [1–3]. Generally, the traditional technologies of capture CO_2 mainly include absorption, adsorption, membrane and cryogenic processes [2]. Amine solutions, as one of the commercialized technologies, are currently the most viable absorbents for CO_2 capture. However, the main technical barriers to the large-scale application of these technologies are the issue of significant energy penalty, which have been mentioned in the research of CO_2 absorption [4–6] and CO_2 adsorption [7,8].

Adsorption technology is recognized to be a promising CO_2 capture method available to the small and medium scale CO_2 emitters due to the reusable nature of adsorbents, low capital investment and easy automatic operation [9]. In addition, adsorption technologies can be widely used in various fields, such as adsorption chillers [10] and energy storage systems [11]. Within the category of adsorption processes, pressure swing adsorption (PSA) and temperature swing adsorption (TSA) are considered as effective alternatives to remove CO_2 from the other components in flue gas. Focusing on pressure swing adsorption cycles, the feeding gas system operates at a pressure higher than atmospheric pressure by air compressor, resulting in significant energy consumption, because higher feeding pressure are directly proportional to higher energy consumption.

Finding the most efficient adsorbents has attracted the focus of both experimental and theoretical research, and even new adsorbent materials are synthesized in large scale, claiming suitability for CO_2 capture. Currently, the choice of adsorbent plays a crucial role on the designing CO_2 adsorption processes [12]. On the one hand, the classical materials, such as zeolite 5A and silica gel, have been studied extensively for CO_2 capture. On the other hand, the novel materials like metal organic frameworks (MOFs) have caught the attention because of the high CO_2 loading capacity and selectivity. As alternatives to amine solutions, zeolites, silica gel, activated carbon and MOF have received significant attention due to the reduced energy consumption.

In the past few years, several research groups worldwide have initiated work on the development of solid sorbents for CO_2 capture. Sjostrom and Krutka [13] have examined twenty-four different sorbent materials on a laboratory scale in TSA process and indicate that the supported amines exhibited the highest CO_2 working capacities. Wang et al. [14] have reviewed three types of solid CO_2-adsorbents according to their sorption/desorption temperatures: below 200 °C, between 200 and 400 °C and above 400 °C, respectively. Samanta et al. [15] have summarized the present state of knowledge on the solid sorbents with and without nitrogen functionality. Maring and Webley [16] have presented a new simplified pressure/vacuum swing adsorption model which can be used to quickly screen adsorbents for use in CO_2 capture applications. Veneman et al. [17] have studied the adsorption of H_2O and CO_2 on supported amine sorbents (Lewatit VP OC 1065), and both CO_2 and H_2O were found to adsorb on the amine active sites present on the pore surface of the sorbent material. Lee and Park [18] have summarized dry solid adsorbents for CO_2 capture and state that the performances of currently available adsorbents need to be improved in terms of working adsorption capacity, cycle lifetime, and multi-cycle durability. Bahamon and Vega [19] have tested eleven adsorbents for CO_2 separation by systematic evaluation and indicate that Mg-MOF-74 appears the best for the TSA process among the studied materials. As shown in Fig. 1, the current researches mainly focus on the selectivity, stability, capacity, and energy for regeneration, etc. Hence, there are few studies on the energy-efficiency analysis of CO_2 adsorption capture technologies from the point of various adsorbent materials. Some conclusions in published research demonstrated that a blind pursuit without enough theoretical considerations of thermodynamic cycle would lead to misguided research directions for CO_2 capture [20].

According to our previous studies, the theory of thermodynamic carbon pump is applied for the energy-efficiency analysis of CO_2 adsorption capture technologies. Based on literature review, case studies of different CO_2 capture technologies have been widely studied using the theory of thermodynamic carbon pump [21]. In addition, a comparative study on CO_2 capture performance of VPSA and PTSA is conducted using the theory of thermodynamic carbon pump [22]. However, the researches on the effect of different adsorbent materials with respect to VPSA cycles have not been found via literature review.

The main goal of this paper is to investigate the effect of different adsorbent materials on the energy-efficiency performance of VPSA cycles. Firstly, the adsorbent isotherm models of five adsorbent materials, which are Mg-MOF-74, zeolite 13X, zeolite 5A, activated carbon and silica gel, are collected for energy-efficiency analysis of VPSA cycles. Then, the analysis of 5-step VPSA cycle, which includes pressurization, adsorption, depressurization, evacuation and purge, is conducted using the theory of thermodynamic carbon pump from cycle parameters. The energy-efficiency performance of the 5-step VPSA cycles is studied in terms of the minimum separation work, the energy consumption and the second-law efficiency. Finally, the key parameters of the effect on