CHEMICAL ENGINEERING RESEARCH AND DESIGN XXX (2017) XXX–XXX

Contents lists available at ScienceDirect

Chemical Engineering Research and Design

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

A model-based approach for the evaluation of new zeolite 13X-based adsorbents for the efficient post-combustion CO_2 capture using P/VSA processes

George N. Nikolaidis, Eustathios S. Kikkinides, Michael C. Georgiadis*

Department of Chemical Engineering, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

ARTICLE INFO

Article history:
Received 3 April 2017
Received in revised form 9 June 2017
Accepted 13 June 2017
Available online xxx

Keywords:
PSA/VSA process
Adsorbents
13X zeolite
CO_2 capture
Dynamic optimization

ABSTRACT

This work presents a mathematical modeling framework for the simulation and optimization of pressure/vacuum swing adsorption (P/VSA) processes for post-combustion CO_2 capture. A single-stage P/VSA process for CO_2 capture from dry flue gas is considered using new zeolite 13X-based adsorbents resulting from perturbation on the 13X zeolite isotherm. A two-bed six-step P/VSA cycle configuration with light product pressurization is employed in systematic simulation and optimization studies. First a zeolite 13X, the current benchmark commercial adsorbent for CO_2 capture, is considered. Accordingly, the model is used to study and evaluate new zeolite 13X-based adsorbents for more efficient CO_2 capture. The results from systematic comparative simulation studies demonstrate that a modified zeolite 13X-based adsorbent appears to have better process performance compared with the original zeolite 13X. Furthermore, process optimization studies employing the above potential adsorbents are performed to minimize energy consumption for specified minimum requirements in CO_2 purity and recovery. The optimization results indicate that the minimum target of 95% in CO_2 purity and 90% in CO_2 recovery is easily met for the P/VSA process under consideration for both potential adsorbents under different operating conditions resulting in different energy requirements and CO_2 productivity.

1. Introduction

Carbon dioxide (CO_2) emissions are considered as a great threat to the environment because they are responsible for 60% of the global warming caused by greenhouse gases (GHGs). Fossil fuels constitute currently the dominant energy source because of their availability and low cost and are expected to retain this dominance during the next decades. Therefore, carbon capture and storage (CCS) from several energy intensive industrial processes will play a critical role in the production of a significant proportion of energy from fossil fuels, enabling reduced GHGs emissions, and improving the security of supply by maintaining a balanced mix of energy sources. The first step in CCS is CO_2 capture at the source and the production of a concentrated stream for pressurization, liquefaction, transportation and storage in potential reservoirs. CO_2 capture is the most expensive part of CCS accounting for 70–80% of the overall CCS cost (Lee and Park, 2015). Currently, there are three main available approaches to capture CO_2 from large scale industrial facilities or power plants: (1) post-combustion capture, (2) pre-combustion capture, and (3) oxy-fuel combustion capture. Post-combustion capture involves the separation and capture of CO_2 from large exhaust sources including coal-fired power plants, cement industries, iron and steel mills and other industrial sectors. Pre-combustion capture involves first the gasification or reforming of solid, liquid or gaseous fuel into syngas, which is a combustible fluid mixture

---

Abbreviations: CFDM, centered finite difference method; PDAEs, partial differential and algebraic equations; PSA, pressure swing adsorption; P/VSA, pressure vacuum swing adsorption; SLPM, standard liters per minute; TSA, temperature swing adsorption; VSA, vacuum swing adsorption.

* *Corresponding author.*

E-mail address: mgeorg@auth.gr (M.C. Georgiadis).

http://dx.doi.org/10.1016/j.cherd.2017.06.016
0263-8762/

Please cite this article in press as: Nikolaidis, G.N., et al., A model-based approach for the evaluation of new zeolite 13X-based adsorbents for the efficient post-combustion CO_2 capture using P/VSA processes. Chem. Eng. Res. Des. (2017), http://dx.doi.org/10.1016/j.cherd.2017.06.016

Nomenclature

$b_{(1)}$	Dual site Langmuir isotherm parameter of first site, 1/Pa
$b_{(2)}$	Dual-site Langmuir isotherm parameter of second site, 1/Pa
C	Molar concentration of gas phase in bulk gas, mol/m^3
C^{in}	Molar concentration of gas phase at the inlet of adsorption bed, mol/m^3
c_p	Specific heat capacity of bulk gas referring to constant pressure, J/(kg K)
c_v	Specific heat capacity of bulk gas referring to constant volume, J/(kg K)
c_p^p	Specific heat capacity of the particle, J/(kg K)
C_{valve}	Gas valve constant
D	Adsorption bed diameter, m
D_e	Effective diffusivity, m^2/s
D_k	Knudsen diffusivity, m^2/s
D_m	Molecular diffusivity, m^2/s
D_z	Axial dispersion coefficient, m^2/s
E	Energy consumption of the compressor/vacuum pump, J
F	Molar flow rate, mol/s
$k_{1(1)}$	Dual-site Langmuir isotherm parameter of first site, mol/kg
$k_{2(1)}$	Dual-site Langmuir isotherm parameter of first site, 1/K
$k_{3(1)}$	Dual-site Langmuir isotherm parameter of first site, 1/Pa
$k_{4(1)}$	Dual-site Langmuir isotherm parameter of first site, K
$k_{1(2)}$	Dual-site Langmuir isotherm parameter of second site, mol/kg
$k_{2(2)}$	Dual-site Langmuir isotherm parameter of second site, 1/K
$k_{3(2)}$	Dual-site Langmuir isotherm parameter of second site, 1/Pa
$k_{4(2)}$	Dual-site Langmuir isotherm parameter of second site, K
$k_{h,wall}$	Heat transfer coefficient of the bed wall, J/(m^2 K s)
L	Adsorption bed length, m
MW	Molecular weight, g/mol
N_{comp}	Number of components
N_{in}	Number of moles of the feed stream of the compressor/vacuum pump, mol
n_c	Isentropic compression efficiency of the compressor
n_v	Isentropic evacuation efficiency of the vacuum pump
P	Total pressure of bed, Pa
P_{atm}	Atmospheric pressure, Pa
P_{factor,CO_2}	CO_2 perturbation factor of the dual-site Langmuir isotherm parameters
P_{factor,N_2}	N_2 perturbation factor of the dual-site Langmuir isotherm parameters
P_{feed}	Pressure of the feed stream, Pa
P_{in}	Pressure at the inlet of the gas valve, Pa
P_{out}	Pressure at the outlet of the gas valve, Pa
P_v	Pressure of the leaving stream of the vacuum pump, Pa
Q	Adsorbed amount per unit mass of adsorbent, mol/kg
Q*	Adsorbed amount per unit mass of adsorbent in equilibrium state, mol/kg
q_m	Dual-site Langmuir isotherm parameter, mol/kg
R_{bed}	Adsorption bed radius, m
R_p	Particle radius, m
R_{pore}	Pore radius, m
SP	Stem position of the gas valve
t	Time, s
t_{Ads}	Time of adsorption step, s
t_{Blow}	Time of blowdown step, s
t_{Evac}	Time of evacuation step, s
t_{cycle}	Total cycle time step, s
t_{CC}	Time of pressurization with light product step, s
t_{PED}	Time of pressure equalization (depressurization) step, s
t_{PER}	Time of pressure equalization (repressurization) step, s
T	Temperature of the adsorption bed, K
T_{feed}	Temperature of the feed stream, K
T^{in}	Temperature of the fluid at the inlet of the adsorption bed, K
T_{wall}	Temperature of the bed wall, K
u	Interstitial velocity, m/s
u^{in}	Interstitial velocity at the inlet of the adsorption bed, m/s
y	Molar fraction in gas phase
z	Axial discretization domain, m

Greek letters

γ	Specific heat capacity ratio
ΔH_{ads}	Isosteric heat of adsorption, J/mol
ε_{bed}	Porosity of the adsorption bed
ε_p	Porosity of the particle
λ	Thermal conductivity of bulk gas, J/(m K s)
λ_z	Heat axial dispersion coefficient, J/(m K s)
μ	Viscosity of bulk gas, Pa s
ρ	Density of bulk gas, kg/m^3
ρ^p	Density of the particle, kg/m^3
ρ^s	Adsorbent density, kg/m^3
τ_p	Tortuosity factor of the particle

Subscripts

i	Component

Superscripts

p	Particle

containing CO_2. CO_2 is separated from syngas before combustion. The syngas is then burned in a conventional combined-cycle arrangement integrated to the gasification unit (Integrated Gasification Combined Cycle, IGCC) to generate electric power. In oxy-fuel combustion the fuel is burned with oxygen instead of air, to produce a flue gas that consists of primarily CO_2. The National Energy Technology Laboratory, under the U.S. Department of Energy, has specified 95% CO_2 purity and 90% CO_2 recovery target levels for the CO_2 capture processes (NETL, 2012). According to the International Energy Agency's roadmap, 20% of the total CO_2 emissions should be removed by CCS by the year 2050

Please cite this article in press as: Nikolaidis, G.N., et al., A model-based approach for the evaluation of new zeolite 13X-based adsorbents for the efficient post-combustion CO_2 capture using P/VSA processes. Chem. Eng. Res. Des. (2017), http://dx.doi.org/10.1016/j.cherd.2017.06.016