Effect of monolithic structure on CO_2 adsorption performance of activated carbon fiber–phenolic resin composite: A simulation study

Hui An [a], Bo Feng [a,*], Shi Su [b]

[a] School of Mechanical & Mining Engineering, The University of Queensland, St. Lucia, QLD 4072, Australia
[b] CSIRO, PO Box 883, Kenmore, QLD 4069, Australia

ABSTRACT

Activated carbon fiber–phenolic resin composite, which has a form of honeycomb monoliths, has been used to capture CO_2. A theoretical model was proposed and utilized to predict the sample's breakthrough curves under various structural conditions to study the relationship between the sample's monolithic structure and its adsorption performance. Three geometric factors including number of channels, internal channel diameter and sample's diameter were chosen to vary while the sample's weight was kept constant. It is found that the sample's adsorption performance increases proportionally with the increase of its void fraction. The sample with thinner channel walls also achieves better adsorption performance. As far as the optimal structure is concerned, the effect of the sample's diameter is considered negligible as long as the void fraction is maintained. By increasing either the number of channels or internal channel diameter, the sample's adsorption performance can be improved. However, a smaller channel size is preferred due to its potential in reducing the sample size. More channels thus have to be made to achieve a certain void fraction.

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1. Introduction

Fossil fuel-fired power plants are large sources of CO_2 emissions. A lot of research has been undertaken for CO_2 removal from the flue gas of power plants and efforts are also being made to bring down CO_2 capture cost to make the abatement of CO_2 emissions more economical. Previously, we reported an adsorbent named activated carbon fiber–phenolic resin composite [1]. This material demonstrates better CO_2 adsorption performance than a series of sorbents, for example, granular activated carbon. Therefore, it has a potential to capture CO_2 more energy efficiently. Another advantage of activated carbon fiber–phenolic resin composite is its flexibility to be made into any shapes. The activated carbon fiber–phenolic resin composite investigated in this work takes the structure of honeycomb monoliths as introduced in more detail in Section 2.1. This honeycomb monolithic form enables the material to have good attrition properties and low pressure drops which prove to be paramount in adsorption applications.

Materials in a honeycomb monolithic form have been investigated for many applications, especially in automotive catalyst carriers [2–4] and de-NO_x SCR catalysis [5–7]. Activated carbon fiber–phenolic resin in the form of honeycomb monoliths has been designed specifically for CO_2 capture from fossil fuel-fired power plants, including coal fired power plants. In the flue gas from coal fired power plants, however, there is a large content of ash and dust. Monolithic catalysts have demonstrated their capabilities to be used in the selective catalytic reduction (SCR) of NO_x in both low and high dust environments in power plants [5,7]. Monolithic materials also found applications in adsorption. Grande et al. [8] provides an elaborate list of studies on gas phase adsorption using monolithic materials in their paper which focuses on adsorption of propane and propylene in zeolite 4A honeycomb monolith. The structural parameters of the monolith are known to have an effect on its adsorption performance. Gadkaree [9] studied the influence of structural parameter channel wall thickness on adsorption performance of activated carbon honeycombs. It is found that when two samples have the same cell density and length, the sample with thicker walls shows improved adsorption performance when both samples are exposed to the adsorbate under identical conditions. However, Gadkaree points out that the amount of carbon on the thick-walled sample is more than that in the thin-walled sample. And the 52% increase in carbon results in a 46% increase in adsorption capacity. Valdes-Solis et al. [10] analyzed n-butane breakthrough curves on carbon-coated ceramic monoliths and found that stacking of the monolithic pieces, increasing cell density and gas redistribution between pieces improve the breakthrough performance. The influence of weight change in these tests is not reported. Therefore, there is an interest to investigate the effects of structural parameters of monolith on its adsorption performance on a weight basis.

Nomenclature

a_p	specific area per volume (1/m)
C	CO_2 concentration in gas phase (mol/m^3)
C_0	inlet concentration in gas phase (mol/m^3)
C_{sat}	saturation concentration at T (mol/m^3)
D	characteristic length ($=D_{in}$) (m)
D_{ax}	axial dispersion coefficient (m^2/s)
D_{eff}	effective diffusivity (m^2/s)
D_{in}	internal diameter of the channel (m)
D_K	Knudsen diffusivity (m^2/s)
D_{mol}	molecular diffusivity (m^2/s)
D_{out}	outer diameter of the channel (m)
D_{sam}	diameter of the sample (m)
E	activation energy (J/mol)
k	Henry constant
k_f	mass transfer coefficient (m/s)
L	average pore size (nm)
L_c	length of the channel (m)
MW	molecular weight of CO_2 (g/mol)
n_{ch}	number of channels
q	instantaneous amount of CO_2 adsorbed (mol/m^3)
q'	amount of CO_2 in equilibrium at C^w (mol/m^3)
q_{max}	amount of CO_2 in equilibrium at C_{sat} (mol/m^3)

r	radial position in the channel
R	gas constant (J/mol/k)
Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number
t	time (s)
T	adsorption temperature (K)
v_{ch}	flow velocity in the channel (m/s)
W_{th}	wall thickness of the channel, $(D_{out}-D_{in})/2$ (m)
z	distance from the inlet of the channel (m)

Subscripts and superscripts:

w	channel wall
$*$	gas–solid interface

Greek letters:

ε_m	void fraction of the monolith
ε_w	porosity in the monolith wall
ρ	gas phase density (g/m^3)
ρ_c	cell density of the monolith ($1/cm^2$)
μ	gas viscosity (g/m/s)

In this work, activated carbon fiber–phenolic resin composite has been investigated for CO_2 adsorption and it takes a honeycomb monolithic structure due to the good attrition properties, low pressure drop and high resistance to dust. A theoretical model was proposed to predict CO_2 adsorption breakthrough curves of activated carbon fiber–phenolic resin composite in order to study its adsorption performance. The model was then utilized to investigate the relationship between the sample's monolithic structure and its adsorption performance. The aim was to design the composite with an optimal structure in an attempt to maximize its CO_2 adsorption performance when its weight remains unchanged.

2. Experiment

2.1. Material

The material investigated for CO_2 adsorption is activated carbon fiber–phenolic resin composite. The detailed fabrication procedure is described as follows [1,11–13]. Milled pitch-based carbon fibers and powdered phenolic resin were mixed in a mass ratio of 2:1. Water was then added to form a water slurry. After mixing well, the water slurry was transferred to a molding tank with 17 evenly distributed Teflon poles inside. Water was removed by vacuum pumping through a filter at the bottom of the tank. The molding tank containing carbon fiber–phenolic resin mixture was then placed in an oven and went through overnight drying at 70 °C and subsequent curing at 130 °C for 2 h. The sample was thus solidified. After cooling down, the sample, which took the cylindrical form of the molding tank, was taken out. By carefully removing 17 Teflon poles, 17 elongated channels were made in the sample. The sample was then carbonized at 650 °C under N_2 flow for 3 h and activated by CO_2 at 900 °C for 5.5 h in a tube furnace. A burn-off of 31.1% was achieved. The final sample has a cylindrical form of 7.62 cm length and 3.03 cm diameter. The elongated channels have a circular section of 0.3 cm in diameter.

TriStar 3000 (Micrometritics) was employed to analyze the porous structure of the sample. The sample's BET surface area obtained by N_2 adsorption isotherm at −196 °C is 998 m^2/g. Adsorption properties of activated carbon fiber–phenolic resin

composites have been discussed in a previous paper [1]. Additionally, desorption of CO_2 from the composite by electrothermal effect has been investigated and reported [14]. It has been found that desorption efficiency above 90% can be easily accomplished in each test. The ad-/desorption performance of the sample investigated remained after 90 ad-/desorption cycles, although further research is needed to test the reusability of this composite.

2.2. Equilibrium isotherm

The adsorption equilibrium isotherm data of CO_2 in activated carbon fiber–phenolic resin composite was obtained with the application of TriStar 3000. Fig. 1 shows the adsorption isotherms at 0 °C and 25 °C. It can be seen that more CO_2 is adsorbed when pressure increases or temperature decreases. An increase in the adsorption temperature from 0 °C to 25 °C under atmospheric pressure sees the amount of CO_2 adsorbed drop from 4.3 mmol/g to 2.7 mmol/g, by 37%. Dubinin-Radushkevich (DR) method has
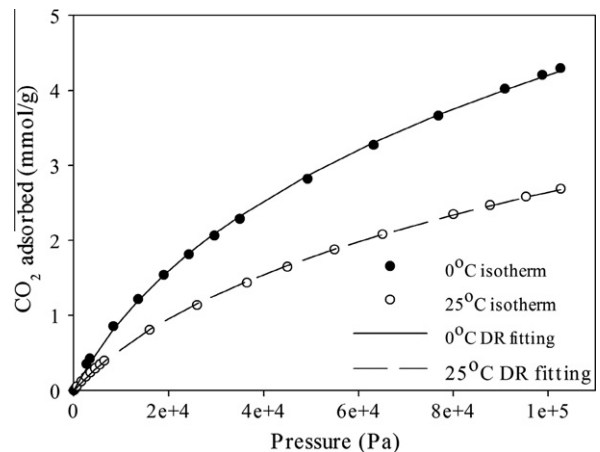

Fig. 1. CO_2 adsorption isotherms with DR fittings.