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Carbon dioxide and nitrogen adsorption on porous copolymers of divinylbenzene and acrylic acid

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Abstract Porous copolymers of divinylbenzene (DVB) and acrylic acid (AA) having DVB:AA ratios of 6:4, 8:2 and 9:1 were prepared following a distillation-precipitation method, using toluene as the porogenic agent. The materials thus obtained, which showed specific surface area in the range of 380–600 $m^2\ g^{-1}$ and pore volume in the range of 0.14–0.18 $cm^3\ g^{-1}$, were investigated as possible adsorbents for CO_2 capture from the flue gas of coal-fired power stations. For that purpose, the isosteric heat of adsorption (and CO_2 adsorption capacity) was analysed from N_2 and CO_2 adsorption equilibrium isotherms obtained over a temperature range. For CO_2, q_{st} resulted to be in the range of 27–31 kJ mol^{-1} (the highest value corresponding to the 6:4 sample), while for N_2 a value of $q_{st} \approx 12$ kJ mol^{-1} was obtained. Equilibrium adsorption capacity for CO_2 (at ambient temperature and pressure) showed the value of about 1.35 mmol g^{-1}. These results are discussed in the broader context of corresponding literature data for CO_2 capture using protonic zeolites.

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1 Introduction

Oil, natural gas and coal, taken together, account for about 80 % of present-day primary energy supply (Van den Berg and Arean 2008). These three carbon-based energy sources (collectively known as fossil fuels) rendered possible the rapid development of our technological civilization that lead to the present level of well-being and comfort. However, CO_2 vented to the atmosphere when burning these fossil fuels in power stations constitutes a major factor of ever increasing greenhouse effect and consequent concern about potential adverse effects on climate change. Replacing fossil fuels with cleaner, and renewable, energy sources would provide a way out of this situation in the long run. However, the current high cost of implementing new technologies for electric energy production, added to worldwide increasing energy demand, calls for a mid-term solution to allow the humanity to continue using fossil fuels until cost-effective renewable energy can be implemented on a large scale. Carbon dioxide capture and sequestration (CCS) could constitute part of that mid-term solution, particularly if current research in this area brings about a significant cost reduction.

Implementation of CCS from the flue gases of fossil-fuel power plants can be accomplished by means of amine-based (or ammonia based) chemical absorbents (Aaron and Tsouris 2005; Rochelle 2009; Strube et al. 2011), but recycling these CO_2 absorbents on a large scale can increase the cost of energy production by as much as 70 % (Haszeldine 2009) and, besides that, accidental spills can pose environmental hazards (Thitakamol et al. 2007; Karl et al. 2011); hence the convenience to search for less expensive and safer CO_2-capturing media. Among them, porous solids capable of separating CO_2 from flue gases by (reversible) physical adsorption (instead of chemical absorption) constitute a main topic of current research in this field.

Main types of porous materials currently under active research for CO_2 separation from flue gases of power stations are porous carbons (Dreisbach et al. 1999; Arenillas et al. 2005; Gutierrez et al. 2011; Schell et al. 2012; Wang et al. 2012), metal–organic frameworks (MOFs) (Martin-Calvo et al. 2012; Ramsahye et al. 2007; Laissig et al. 2011; Bae and Snurr 2011; Valenzano et al. 2010) and zeolites (Xiao et al. 2008; Garcia-Sanchez et al. 2009, Grajciar et al. 2012, Delgado and Arean 2011; Arean et al. 2011, 2012). However, less reports seem to be available for CO_2 capture in porous organic polymers (Dawson et al. 2011; Furukawa and Yaghi 2009; Katsoulidis and Kanatzidis 2011). It should be noted that the ideal properties of the most convenient CO_2 adsorbent will depend on the particular process for which it is intended. Thus, in post-combustion capture CO_2 has to be separated from a flue gas that contains about 15 % of CO_2 and 85 % of N_2, and also a non-negligible amount of water vapour; while in pre-combustion capture of CO_2 the stream (H_2, CO and CO_2) usually contains a higher proportion of CO_2 (about 35 %), and the process should be implemented at a higher temperature and pressure than in the case of post-combustion. However, the vast majority of currently operated power stations work under a post-combustion regime, which would require CO_2 capture at ambient pressure from flue gases containing some water vapour; and that renders the use of MOFs rather problematic, in view of their well known hydrolytic instability.

We report herein on carbon dioxide and dinitrogen adsorption (up to ambient pressure) on porous polymers obtained by copolymerization of divinylbenzene (DVB) and acrylic acid (AA). N_2 and CO_2 adsorption isotherms (at 77 and 273 K, respectively) were used for textural characterization and for determination of CO_2 adsorption capacity; followed by determination of isosteric heats of adsorption from gas adsorption isotherms obtained over a temperature range. The results obtained are discussed in the broader context of dinitrogen and carbon dioxide adsorption in protonic zeolites.

2 Experimental

2.1 Copolymer synthesis

Porous poly(DVB-co-AA) polymers having different DVB:AA ratios were synthesized (in the shape of sub-micrometer spherical particles) following a distillation-precipitation method, using toluene as the porogenic agent, acetonitrile as the solvent and 2,2′-azobisisobutyronitrile (AIBN) as the polymerization initiator. Briefly, a 2 mL mixture of DVB and AA (in the appropriate ratio), together with 0.04 g of AIBN, was added to 80 mL of a 4:1 mixture of acetonitrile and toluene contained in an 100 mL two-necked flask attached to a fractionating column, a Liebig condenser and a receiver. The reaction mixture was heated to the boiling point and the process was stopped after 40 mL of the solvent mixture was distilled. The resulting poly(DVB-co-AA) solid was separated by vacuum filtration through a sintered glass filter, successively washed out with acetonitrile and acetone and finally dried in a vacuum oven till constant weight was attained. In separate preparations, poly(DVB-co-AA) samples having a DVB:AA ratio of 9:1, 8:2 and 6:4 were thus obtained. Further details about the general aspects of this synthesis method can be found elsewhere (Liu et al. 2006, 2009). Transmission electron microscopy showed that each poly(DVB-co-AA) polymer sample thus obtained consisted of approximately monodispersed spheres having a diameter of 0.6, 1.8 and 1.9 μm for samples having a DVB:AA ratio of 6:4, 8:2 and 9:1, respectively. Representative electron micrographs are shown in Fig. 1.

2.2 Textural characterization and determination of isosteric heats of adsorption

Textural characterization of the synthesized samples was carried out by measuring the N_2 (ASAP 2020, Micromeritics) and CO_2 (Tristar 3020, Micromeritics) adsorption isotherms at 77 and 273 K, respectively. In order to prevent the degradation of the samples special attention was paid to the degassing pretreatment, prior to gas adsorption measurements. For that purpose all of the samples were carefully outgassed under high vacuum (ca. 10^{-3} Torr) in three steps: (1) outgassing at the rate of 5 Torr/min while heating at the rate of 1 °C/min up to 50 °C, (2) once the pressure was below 10^{-5} Torr, the temperature was kept constant at 50 °C for 1 h, (3) finally, the samples were heated up to 100 °C and outgassed at that temperature for 2 h. The N_2 adsorption isotherms were used to calculate the specific surface area, S_{BET}, and the BET constant, C_{BET}, which is related to the strength of the interactions between the gas and the adsorbent. The distribution of pores smaller than 0.7 nm (narrow microporosity) was assessed from CO_2 adsorption isotherms by applying the DRS equation (Dubinin and Stoeckli 1980) and using 1.023 g cm^{-3} as the density of adsorbed CO_2 and 0.36 as the β parameter.

The isosteric heats of adsorption for N_2 and CO_2 were evaluated from the corresponding gas adsorption isotherms obtained over a temperature range and using the Clausius-Clapeyron equation (Eq. 1):

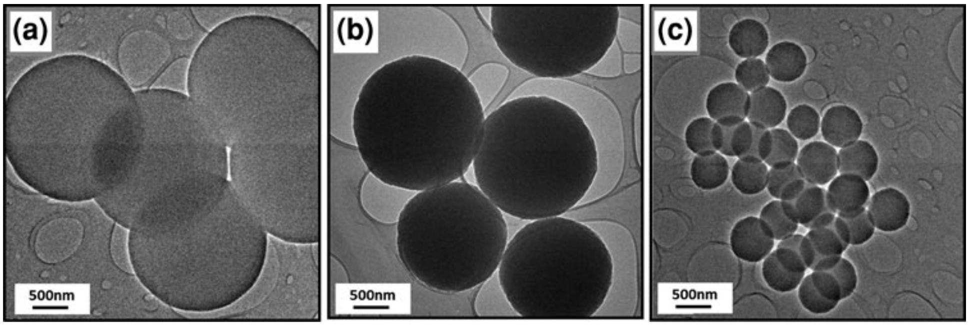

Fig. 1 Representative transmission electron micrographs of the porous polymers: **a** 9:1, **b** 8:2 and **c** 6:4

$$q_{st} = -R\left(\frac{\delta \ln P}{\delta(1/T)}\right)_N \quad (1)$$

where q_{st}, R, P, and N stand for isosteric heat of adsorption, gas constant, pressure, and amount of adsorbed gas, respectively. For that purpose, CO_2 adsorption isotherms were obtained at six fixed temperature values within the range of 258–298 K. In the case of N_2, isotherms were measured at 258, 268 and 278 K. To check the accuracy of the measurements, all of the gas adsorption isotherms were measured in duplicate, and the results were found to be reproducible within an error below 0.1 %.

3 Results and discussion

Adsorption isotherms of N_2 (77 K) and CO_2 (273 K) of the polymer samples are shown in Fig. 2a, b, respectively. The main textural parameters are listed in Table 1. The analysis of the data obtained from the nitrogen adsorption isotherms (Fig. 2a) indicated that all of the materials displayed type I isotherms according to the IUPAC classification (Sing et al. 1985) characteristic of microporous materials. While the isotherms obtained for samples 9:1 and 8:2 are rather similar, giving BET surface areas of 612 and 591 $m^2\ g^{-1}$, respectively, sample 6:4, which gives a BET surface area of 381 $m^2\ g^{-1}$ showed a sharper knee at low relative pressures and a wider hysteresis loop above $p/p_0 = 0.9$ due probably to capillary condensation of the gas inside the interparticle space. These features indicate that, along with a microporous structure comprised of narrow micropores, this sample also exhibits some mesoporosity.

The CO_2 adsorption isotherms at 273 K (Fig. 2b) resulted to be very similar in the three cases, although the sample 6:4, as previously inferred from the corresponding N_2 adsorption isotherm, showed slightly higher CO_2 adsorption up to 600 Torr, indicating the presence of a higher amount of narrow micropores (<0.7 nm). Nevertheless, at higher pressure, the CO_2 isotherms of samples 8:2 and 9:1 closely approach that of the 6:4 sample. These results point to the presence of a larger volume of micropores in the case of the materials with the highest DVB:AA ratio, as reflected in the textural parameters obtained by applying the DRS equation to the CO_2 adsorption isotherms, shown in Table 1. It is also seen in this Table that the S_{BET} value is significantly larger than the corresponding S_{DRS} value for the samples having DVB:AA ratio of 8:2 and 9:1. Likely, the explanation for this observed discrepancy is that the CO_2 adsorption isotherms at 273 K fail to monitor properly the amount of surface area contributed by the wider micropores, which account for the increased mean pore size observed for the two polymer samples having the greater DVB:AA ratio

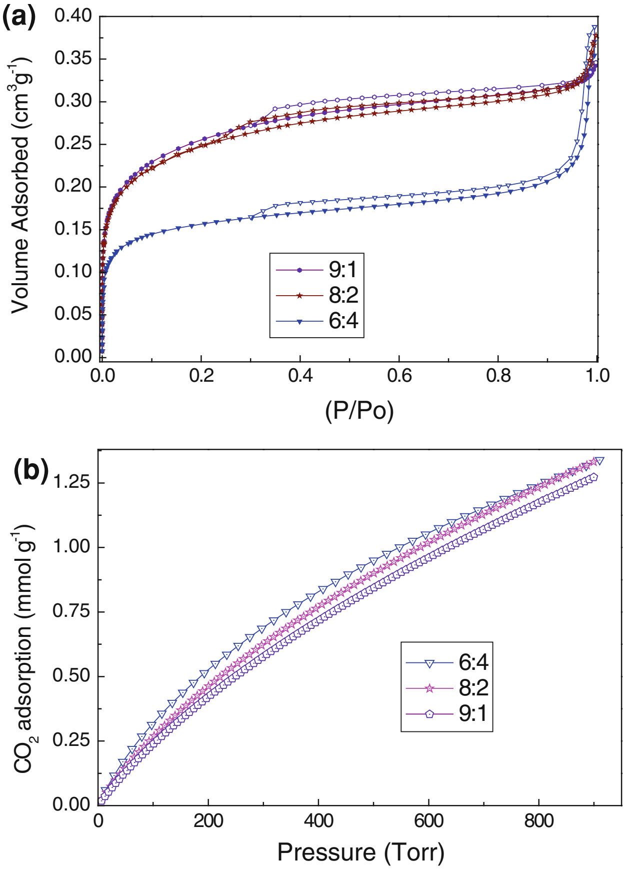

Fig. 2 **a** N_2 Adsorption–desorption isotherms at 77 K on the synthesized porous polymers. **b** CO_2 Adsorption isotherms at 273 K on the synthesized porous polymers

Table 1 Textural parameters of the different poly(DVB-co-AA) porous polymers obtained from N_2 and CO_2 adsorption isotherms at 77 and 273 K, respectively

Sample	DRS applied to CO_2 adsorption isotherm at 273 K				BET applied to N_2 adsorption isotherm at 77 K	
	W_0 ($cm^3\ g^{-1}$)	D_0 (nm)	E_0 (kJ mol^{-1})	S_{DRS} ($m^2\ g^{-1}$)	S_{BET} ($m^2\ g^{-1}$)	C_{BET}
6:4	0.144	0.43	21.6	377	381	282
8:2	0.173	0.56	19.6	453	591	200
9:1	0.177	0.61	19.0	463	612	176

(note also the initial difference in the curvature of the corresponding N_2 adsorption isotherms at 77 K, when compared to that of the 6:4 sample).

Figure 3 shows the isosteric heat of adsorption of CO_2 for the three samples, 9:1, 8:2 and 6:4. At $\theta \rightarrow 0$, q_{st} takes values in the range 27–31 kJ mol^{-1}, which increase with increasing content of acrylic acid. As the amount of adsorbed CO_2 is raised, the isosteric heat of adsorption steadily decreases for all of the studied samples. Regarding the isosteric heat of adsorption of N_2, because of the low adsorption capacity for this gas at room temperature, only the sample 9:1 could be measured (Fig. 3); an approximate value of $q_{st} \approx 12$ kJ mol^{-1} was obtained, which is less than one half of the corresponding value obtained for CO_2 (27 kJ mol^{-1}). This fact, taken together with the very small retention of N_2 observed at room temperature, would ensure that CO_2 can be separated from N_2 with a very high selectivity using these poly(DVB-co-AA) porous polymers.

Regarding the isosteric heats of adsorption of CO_2 on poly(DVB-co-AA) porous polymers, more insight can be obtained by comparison with CO_2 adsorption on protonic zeolites in which the Si(OH)Al group, which acts as a localized adsorbing site for (hydrogen bonded) CO_2, has a Brønsted acidity character similar to that of the acid OH group in acrylic acid. Thus, the observed increasing value of q_{st}, when the AA content in the poly(DVB-co-AA) polymers is increased (Fig. 3), can be explained in terms of a larger proportion of acidic OH groups made accessible inside the pores of the polymer. But, it should also be taken into account that recent studies on CO_2 adsorption in zeolites, which combined DFT/CC calculations with experimental determination of the enthalpy of CO_2 adsorption (ΔH^0) by variable temperature IR (VTIR) spectroscopy (Arean et al. 2002; Garrone and Arean 2005), have shown that, besides localized OH···OCO interactions, there is also a very significant role of weak (delocalized) intermolecular interactions between CO_2 and the zeolite framework, which were found to account for (at least) one half of the observed ΔH^0 value (Pulido et al. 2009; Nachtigall et al. 2012). It seems reasonable to assume that such non-localized interactions should also take place between adsorbed CO_2 and the pore walls of the poly(DVB-co-AA) polymers, and that would reduce the role played by the localized OH···OCO interaction, leading to a concomitant reduced role of the DVB:AA ratio in the corresponding value of ΔH^0 (or q_{st}). The fact that the q_{st} value (Fig. 3) is not seen to show a pronounced decrease when the amount of adsorbed CO_2 is increased would also be consistent with this interpretation.

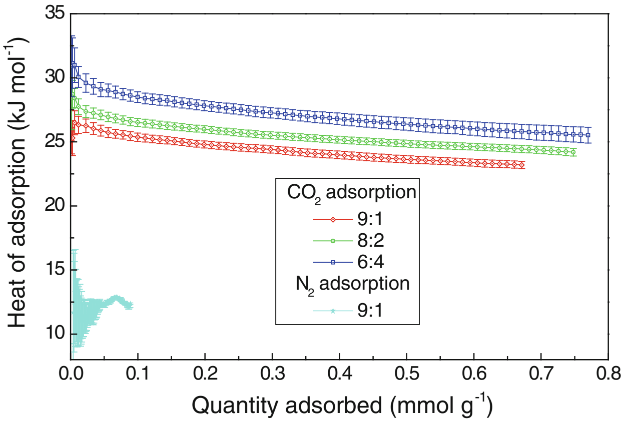

Fig. 3 Isosteric heat of adsorption of CO_2 and N_2 on the poly(DVB-co-AA) porous polymers

Finally, Table 2 summarizes relevant ΔH^0 values reported by several authors for the adsorption of N_2 and CO_2 on protonic zeolites, to be compared with those reported herein for adsorption on poly(DVB-co-AA) porous polymers. For the adsorption of CO_2, the ΔH^0 (q_{st}) values of the porous polymers reported herein are as high as those shown by protonic zeolites, while the adsorption enthalpy of N_2 appears to be significantly smaller for the polymers; which should give these latter adsorbents an advantage regarding CO_2 separation selectivity using pressure (or temperature) swing cycles. Regarding CO_2 adsorption capacity, the value of about 1.35 mmol g^{-1} (at ambient temperature and pressure) found for the poly(DVB-co-AA) porous polymers compares well with that of 1.4 mmol g^{-1} reported in the literature for H-ZSM-5 (Wirawan 2009). Higher values (ranging from 2.5 to 4.7 mmol g^{-1}) were reported for alkaline zeolites (Chue et al. 1995; Lee et al. 2002; Cavenati et al. 2004; Liu et al. 2011); but the CO_2 adsorption capacity of these latter materials becomes greatly reduced by moisture present in

Table 2 Adsorption enthalpy (kJ mol^{-1}) of N_2 and CO_2 on protonic zeolites and on porous poly(DVB-co-AA) polymers

Adsorbed gas	Adsorbent	$-\Delta H^0$	Method[a]	Reference
N_2	H-Beta zeolite	19	VTIR	Delgado and Arean 2011
	H-ZSM-5	19.7	VTIR	Arean 2008
	H-FER	19.1	VTIR	Nachtigall et al. 2009
	H-Y	15.7	VTIR	Arean and Delgado 2010
	9:1 DVB-co-AA	12	q_{st}	This work
CO_2	H-Beta zeolite	33	VTIR	Delgado and Arean 2011
	H-ZSM-5	31.2	VTIR	Armandi et al. 2009
	H-ZSM-5	28.8	q_{st}	Yamazaki et al. 1993
	H-ZSM-5	28.7	q_{st}	Wirawan and Crease 2006
	H-ZSM-5	32–35	CP	Harlick and Tezel 2004
	H-FER	30	VTIR	Pulido et al. 2009
	H-Y	28.5	VTIR	Arean and Delgado 2010
	H-Y	27	q_{st}	Pires et al. 1993
	9:1 DVB-co-AA	27	q_{st}	This work
	8:2 DVB-co-AA	28	q_{st}	This work
	6:4 DVB-co-AA	31	q_{st}	This work

[a] *VTIR* variable temperature IR spectroscopy, q_{st} isosteric heat of adsorption, *CP* chromatography pulse techniques

flue gases (Harlick and Sayari 2006; D'Alessandro et al. 2010), thereby needing regeneration at high temperature, which would significantly increase corresponding costs.

4 Conclusions

Adsorption of carbon dioxide on poly(DVB-co-AA) porous polymers involves an isosteric heat (q_{st}) in the range of 27–31 kJ mol^{-1}, while the value of $q_{st} \approx 12$ kJ mol^{-1} was obtained for N_2 adsorption. The observed large difference between the corresponding q_{st} values should facilitate thermodynamic separation of CO_2 from N_2 in flue gases of coal-fired power stations by pressure-swing adsorption under equilibrium conditions. The adsorption capacity of the porous polymers for carbon dioxide (at ambient temperature and pressure) was found to be of about 1.35 mmol g^{-1}, which compares well with the value of about 1.40 mmol g^{-1} reported in the literature for the protonic zeolite H-ZSM-5. Moreover, since it should be possible to increase pore volume, and hence adsorption capacity, by appropriate design of the synthesis (and composition) of porous polymers, the results shown herein suggest that this kind of physical adsorbents deserve further investigation in the context of carbon dioxide capture from the flue gas of power stations.

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