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Adsorption Equilibrium of Carbon Dioxide and Water Vapor on Zeolites 5A and 13X and Silica Gel: Pure Components

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Adsorption isotherms are reported for pure carbon dioxide and water vapor on 5A and 13X zeolite beads and silica gel granules. These data were obtained using a volumetric method and cover the temperature ranges of (−45 to 175) °C for carbon dioxide and (0 to 100) °C for water. Also, pure carbon dioxide isotherms on silica gel at temperatures from (10 to 55) °C were measured using a gravimetric apparatus. All pure component equilibria are described well by Toth isotherms with parameters having temperature dependence. For carbon dioxide adsorption, zeolites 5A and 13X have similar loadings and show a much higher capacity than silica gel. However, for water vapor, zeolite 13X has a slightly higher capacity than zeolite 5A. Both zeolites have very good adsorption capacities for water vapor at low pressures but lose their advantages to silica gel when water pressures are high.

Introduction

The removal of carbon dioxide and water vapor from air is receiving increasing attention because of emerging needs in air separation, purification, and environmental protection applications. For the conventional cryogenic separation of air, the existence of humidity and carbon dioxide in the air will not permit distillation because the freezing points of H_2O and CO_2 are well above the cryogenic temperature of liquid air. For noncryogenic processes such as pressure swing adsorption (PSA), water vapor and carbon dioxide will detrimentally affect the capacity of adsorbents used for separation or purification.[1] Moreover, a growing need is encountered in applications such as VOC removal, natural gas drying to improve heating value, and space craft atmosphere revitalization systems.[2]

To better design these applications, adsorption equilibrium data for water and carbon dioxide are needed over a wide range of temperatures. Also, it is important to choose proper adsorbents for specific applications. The most widely used desiccant to remove water vapor is silica gel because of its large capacity for water and ease of regeneration. Zeolites are selective adsorbents for the removal of carbon dioxide, water vapor, and other impurities from hydrocarbon mixtures. Normally, two adsorption beds or beds with a layer of silica gel followed by one with zeolite are used to remove water and carbon dioxide. Water adsorption on zeolites is strong, and even a trace amount of water vapor passing through a desiccant bed can drastically affect the adsorption of CO_2 by the zeolite.

Pure water vapor and pure carbon dioxide isotherms on zeolites and silica gel have been reported using volumetric and gravimetric methods, most for one or two temperatures[1,3−8] Multitemperature CO_2 adsorption on zeolite 13X and zeocarbon was obtained using a static volumetric method for (0 to 80) °C and pressures up to 102 kPa and was fitted individually with Toth, UNILAN, and Sips models for each temperature.[3] Similarly, water vapor adsorption equilibria were measured for (20 to 80) °C and pressure up to 2.3 kPa, and the data were correlated by Aranovich−Donohue (A−D) and *n*-layer BET models for each temperature.[4] Rege et al.[1] used a Micromeritics ASAP 2010 volumetric instrument to measure CO_2 and H_2O on several samples including 13X zeolite at (22 and 70) °C for a low pressure range.

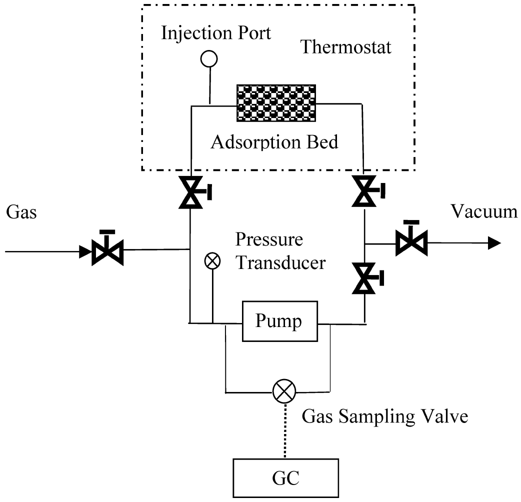

Figure 1. Volumetric adsorption equilibrium apparatus.

In this paper, we report measurements of adsorption isotherms for pure water vapor and carbon dioxide on commercially available 5A and 13X zeolite beads and silica gel over a wide range of temperatures. Experiments were carried out using a volumetric apparatus that includes a high efficiency pump to provide fast circulation for attainment of equilibrium. Single component data are described using a multitemperature Toth model, and five parameters are extracted for each system. Good agreement is shown for all of the systems. Compared to previous research, the multitemperature Toth model has fewer parameters and can describe adsorption equilibrium well within the temperature range studied.

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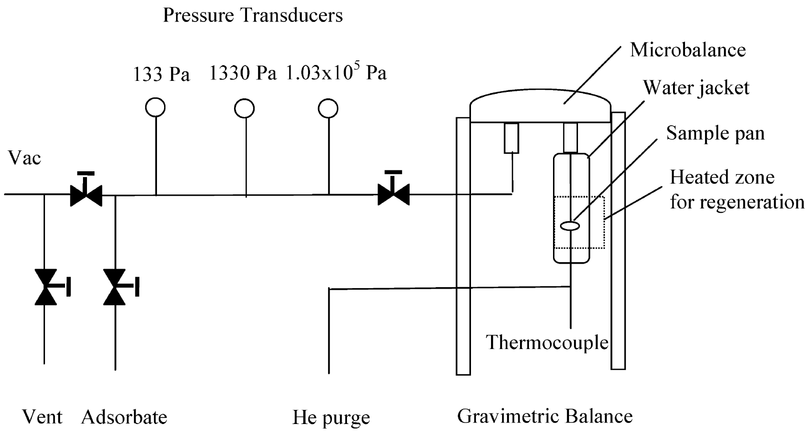

Figure 2. Gravimetric adsorption equilibrium apparatus.

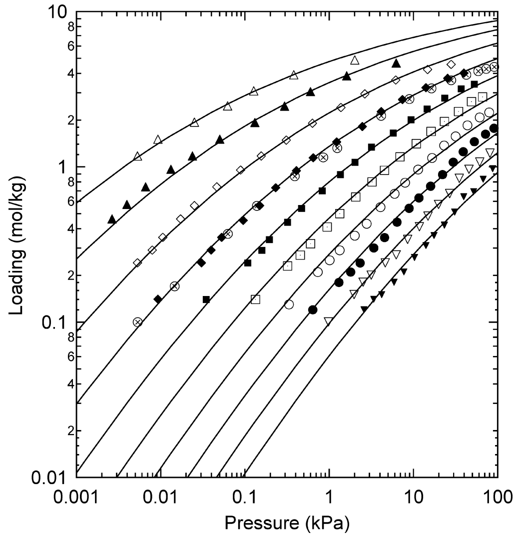

Figure 3. Adsorption isotherms of CO_2 on zeolite 5A: ▼, 175 °C; ∇, 150 °C; ●, 125 °C; ○, 100 °C; □, 75 °C; ■, 50 °C; ◆, 25 °C; ◇, 0 °C; ▲, −25 °C; △, −45 °C; ⊗, 25 °C using gravimetric method; solid curves are Toth isotherms.

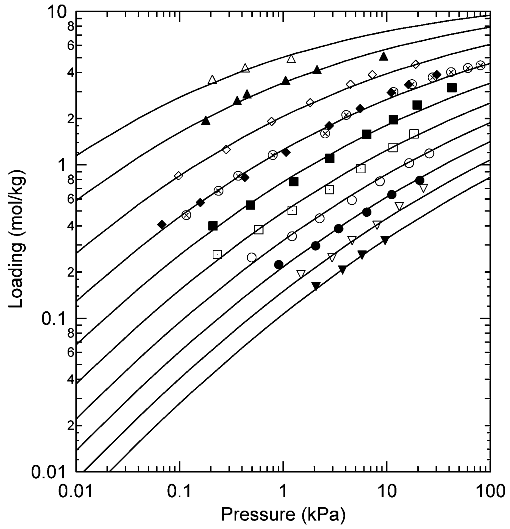

Figure 4. Adsorption isotherms of CO_2 on zeolite 13X: ▼, 175 °C; ∇, 150 °C; ●, 125 °C; ○, 100 °C; □, 75 °C; ■, 50 °C; ◆, 25 °C; ◇, 0 °C; ▲, −25 °C; △, −45 °C; ⊗, 25 °C using the gravimetric method; solid curves are Toth isotherms.

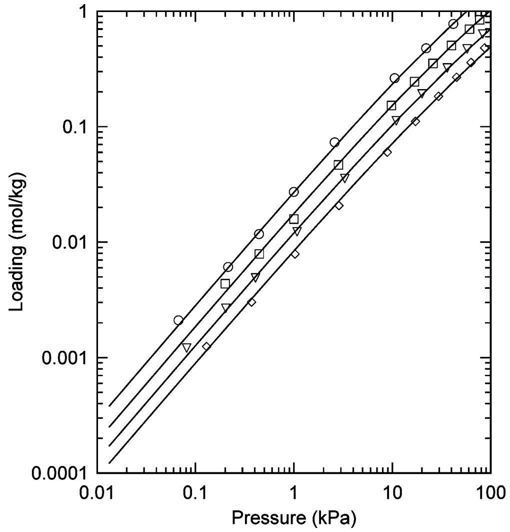

Figure 5. Adsorption isotherms of CO_2 on silica gel: ○, 10 °C; □, 25 °C; ∇, 40 °C; ◇, 55 °C; solid curves are Toth isotherms.

Experimental Section

Materials. The adsorbents used in this study, all manufactured by Grace Davison, were zeolite 5A (MS 522), zeolite 13X (MS 544HP), and silica gel (Grade 40). The zeolites were in the form of 8 × 12 mesh spherical beads. Silica gel was in granular form with very high purity (approximately 99.6 % SiO_2). CO_2 (99.6 %) and helium (99.995 %) were obtained from J&M Cylinder Gases and Air Liquide, respectively.

Apparatus. A volumetric apparatus was constructed to measure adsorption isotherms for pure carbon dioxide and water vapor. A schematic diagram is shown in Figure 1. It is similar to the volumetric apparatus used to investigate coadsorption of water and organic vapors.[9,10] The major difference is that the circulation pump was moved outside of the environmental chamber because of a temperature limitation to allow a wider range of isotherm temperatures to be considered. Only the adsorption bed and injection port were housed in an environmental chamber. The temperature within the chamber could be maintained at a constant value with a precision ± 0.3 °C. Isotherms were measured from (−228 to 448) K, i.e., (−45 to 175) °C.

A known amount of liquid or gas was injected using Hamilton gastight syringes through the injection port and circulated in the closed loop using a magnetic pump.[11] Gas concentrations were sampled and analyzed using a gas chromatograph (HP 6890) to determine when equilibrium was reached. The quantities adsorbed were obtained by material balance knowing the quantity injected and the amount remaining in the vapor phase. It should be emphasized that the amount of adsorbent used and

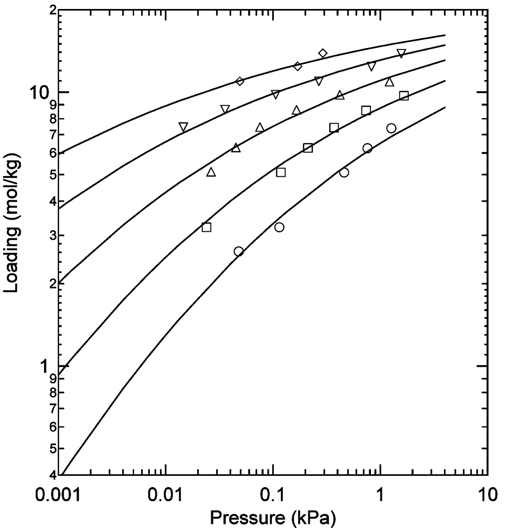

Figure 6. Adsorption isotherms of H_2O on zeolite 5A: ○, 100 °C; □, 75 °C; △, 50 °C; ∇, 25 °C; ◇, 0 °C; solid curves are Toth isotherms.

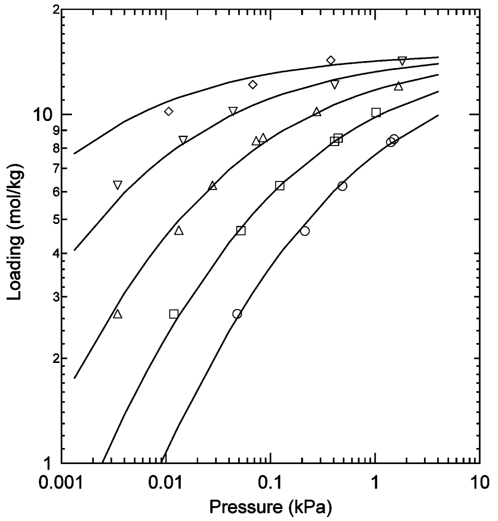

Figure 7. Adsorption isotherms of H_2O on zeolite 13X: ○, 100 °C; □, 75 °C; △, 50 °C; ∇, 25 °C; ◇, 0 °C; solid curves are Toth isotherms.

volume of the loop could be adjusted to retain a large fraction of the injected component in the adsorbed phase with only a small residual amount remaining in the gas phase. In this way, the error in determining the amount adsorbed is small.

We also used a gravimetric apparatus to measure isotherms of pure CO_2 for temperatures from (10 to 55) °C. A schematic diagram of this apparatus is shown in Figure 2. The system combined a Cahn D-200 microbalance with high accuracy pressure transducers operating over different ranges to maintain accuracy. There were two MKS absolute pressure transducers (626A) covering the ranges of $(6.67 \cdot 10^{-2}$ to $1.33 \cdot 10^{2})$ Pa and $(6.67$ to $1.33 \cdot 10^{4})$ Pa with a precision of 0.25 % of reading and one Omega transducer (PX6000) for $(6.90 \cdot 10^{3}$ to $1.03 \cdot 10^{5})$ Pa with a precision of 0.25 % full scale.

Operating Procedures. With the volumetric apparatus, an experiment was begun by regenerating the adsorbent in the environmental chamber at 175 °C under vacuum with dry helium flowing overnight. Then, the desired amount of the single adsorbate was injected into the system, and the temperature was increased to the highest temperature (175 °C for CO_2 and 100 °C for H_2O) for the initial equilibration. Then, the gas-phase concentration in the closed recirculation loop was measured using the gas chromatograph. The temperature was held constant until equilibrium was established as determined by sampling the gas phase. Then, we decreased the system temperature in 25 °C steps, allowed time for equilibration, and measured the gas-phase concentration. The measurements were continued until the lowest temperature was reached. After we finished the measurements for the first CO_2 or H_2O injection, we injected more of the adsorbate into the closed loop and repeated the above procedure until the measurements were completed. A material balance on the system was used to account for all quantities of CO_2 or H_2O added to the circulation loop or removed by sampling.

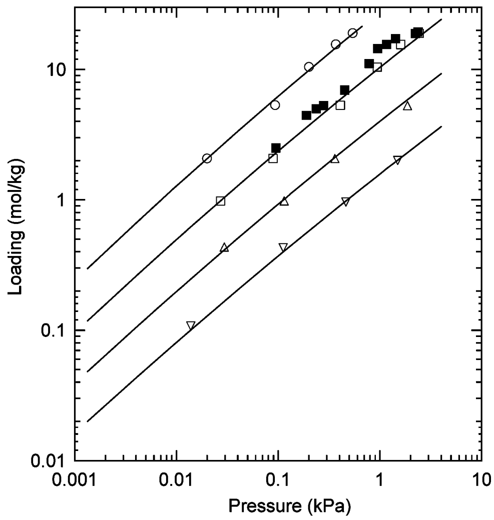

Figure 8. Adsorption isotherms of H_2O on silica gel: ∇, 75 °C; △, 50 °C; □, 25 °C; ○, 0 °C; solid curves are Toth isotherms. ■, Fraioli's data at 20 °C.[5]

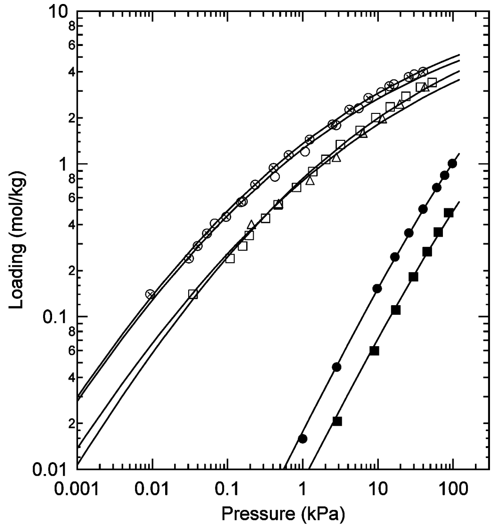

Figure 9. Comparison of CO_2 isotherms on zeolites and silica gel: ○, 25 °C on zeolite 13X; ⊗, 25 °C on zeolite 5A; ●, 25 °C on silica gel; △, 50 °C on zeolite 13X; □, 50 °C on zeolite 5A; ■, 55 °C on silica gel; solid curves are Toth isotherms.

The volumes in the circulation loop inside and outside of the environmental chamber were determined by expansion of helium gas at room temperature. The total system volume inside the environmental chamber was 55.0 cm^3, and the total volume outside of the chamber was 161.8 cm^3. All of the experiments were repeated to confirm the precision of the data.

For the gravimetric experiments, the sample was regenerated in place at 300 °C under vacuum with a helium purge overnight. During the measurement, the temperature was maintained constant by circulating water from a temperature bath through

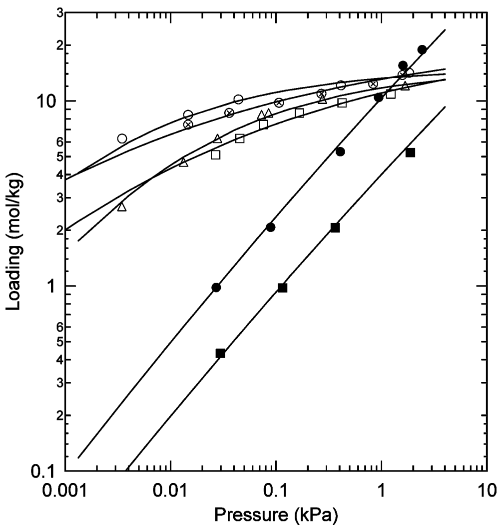

Figure 10. Comparison of H_2O isotherms on zeolites and silica gel: ○, 25 °C on zeolite 13X; ⊗, 25 °C on zeolite 5A; ●, 25 °C on silica gel; △, 50 °C on zeolite 13X; □, 50 °C on zeolite 5A; ■, 50 °C on silica gel; solid curves are Toth isotherms.

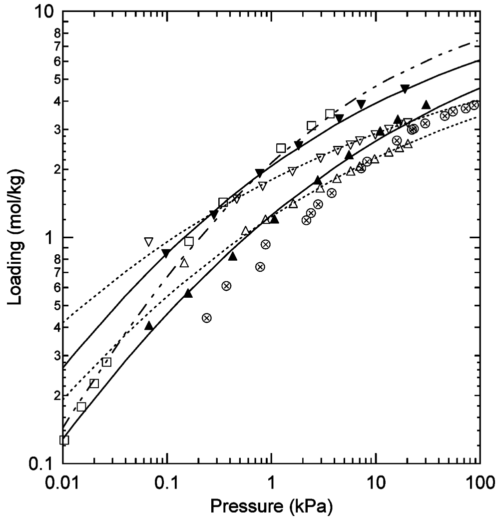

Figure 11. Comparison of adsorption isotherms for pure CO_2 on 13X. Our data: ▼, 0 °C; ▲, 25 °C; solid curves are Toth isotherms). Kim et al.:[3] ∇, 0 °C; Δ, 20 °C; dash curves are Toth isotherms. Rege et al.:[1] □, 22 °C; long short dash curves are Toth isotherms. Hyun and Danner:[6] ⊗, 25 °C.

a water jacket surrounding the sample. CO_2 isotherms at room temperature were measured by both apparatuses to verify the accuracy of the two methods. Except for pure CO_2 adsorbed on silica gel, all other experiments were carried out by the volumetric method.

Results and Discussion

Adsorption isotherms for CO_2 on the zeolites were obtained at temperatures of (−45, −25, 0, 25, 50, 75, 100, 125, 150, and 175) °C and pressures up to 1 bar with the volumetric apparatus. The data are shown in Figures 3 and 4. Both figures also show an isotherm at 25 °C measured using the gravimetric apparatus. The agreement between the two independent methods validates the accuracy of the methods. CO_2 on silica gel was measured using the gravimetric apparatus for temperatures of (10, 25, 40, and 55) °C, and results are shown in Figure 5.

More experiments were carried out with the volumetric apparatus for water vapor isotherms on zeolites 5A and 13X and silica gel at temperatures between (0 and 100) °C and pressures lower than the saturated water vapor pressure at room temperature. These isotherms are shown in Figures 6, 7, and 8. All of the isotherm data of CO_2 and H_2O adsorbed on the zeolites 5A and 13X and silica gel are tabulated in Tables 1 to 7.

Comparing the CO_2 isotherms on zeolites 5A and 13X and silica gel, we find that zeolites 5A and 13X have similar capacities, and silica gel has a lower capacity than both zeolites. Comparison results for (25 and 50) °C are shown in Figure 9. It is clear that CO_2 loadings for silica gel are almost 2 orders of magnitude lower than for zeolites at low pressures and one magnitude lower at high pressures.

However, the results for H_2O isotherms are different, and comparisons for (25 and 50) °C are shown in Figure 10. Zeolite 13X has a slightly better adsorption capacity than zeolite 5A at low pressures. Both zeolites have better water vapor removal ability at low pressures compared to silica gel. With increasing water pressures, silica gel increases in its ability to remove water vapor relative to the zeolites. For example, in comparison to the zeolites, silica gel shows a similar or an increased capability for water removal when the water pressure is above 1 kPa at 25 °C.

For practical utility, the experimental data can be described by an equilibrium model that includes temperature-dependent parameters. The Toth model has a relatively simple form and can effectively describe many systems. Also, it shows correct limiting behavior at low pressures. The Toth equation has three parameters and is of the form

$$n = \frac{ap}{[1 + (bp)^t]^{1/t}} \tag{1}$$

where b is an equilibrium constant; a is a parameter related to b and the saturation capacity; and t characterizes the heterogeneity of the adsorbent. When the surface is homogeneous, the heterogeneity parameter t is equal to unity and the Toth isotherm reduces to the Langmuir isotherm. In applying the Toth equation over a temperature range, the parameters a, b, and t can be considered temperature dependent, with b taking the general form of the adsorption affinity

$$b = b_0 \exp(E/T) \tag{2}$$

a having a similar form

$$a = a_0 \exp(E/T) \tag{3}$$

and t given in terms of reciprocal temperature by

$$t = t_0 + c/T \tag{4}$$

We applied this multitemperature Toth model to describe all of the isotherm data. The isotherms are described well for all temperatures for all systems as shown in Figures 3 to 8. Parameter values are listed in Table 8. The saturation loading can be calculated from the ratio a/b and is considered to be constant for the temperature range. From Table 8, the values of the saturation capacity for CO_2 on zeolite 5A and 13X are (14.6 and 13.3) $mol \cdot kg^{-1}$, respectively, and those for H_2O are (23.5 and 15.1) $mol \cdot kg^{-1}$, respectively. Note that for silica gel the parameters cannot be used to obtain a reliable pore volume capacity because the data do not approach a saturation limit. The multitemperature Toth model has two more parameters, E and c, than the commonly used Toth model with three parameters, which does not consider temperature dependence. Thus, with a Toth model, different values for the three parameters will be obtained for each isotherm, as shown in previous studies.[1,3] In general, the multitemperature Toth model has advantages of fewer parameters and predictive ability for loading at any temperature within the temperature range studied.

Table 1. Adsorption Equilibria of Pure CO_2 on Zeolite 5A Using the Volumetric Method[a]

−45 °C		−25 °C		0 °C		25 °C		50 °C		75 °C		100 °C		125 °C		150 °C		175 °C	
p	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*
0.0053	1.17	0.0027	0.458	0.0053	0.241	0.0093	0.145	0.0347	0.144	0.133	0.139	0.333	0.130	0.640	0.115	0.987	0.100	2.60	0.123
0.0093	1.50	0.0040	0.565	0.0080	0.295	0.0307	0.240	0.108	0.236	0.320	0.226	0.733	0.206	1.31	0.180	1.987	0.150	3.40	0.140
0.0253	1.93	0.0067	0.740	0.0107	0.348	0.0400	0.293	0.159	0.287	0.453	0.273	1.01	0.247	1.80	0.211	2.55	0.177	4.23	0.155
0.0627	2.46	0.0133	0.958	0.0173	0.457	0.0533	0.346	0.195	0.339	0.600	0.320	1.33	0.285	2.33	0.239	3.17	0.202	5.93	0.185
0.128	3.07	0.0240	1.17	0.0253	0.564	0.0960	0.453	0.320	0.442	0.947	0.412	2.01	0.362	3.39	0.298	4.67	0.241	7.76	0.208
0.383	3.90	0.0507	1.50	0.0467	0.738	0.151	0.558	0.471	0.543	1.33	0.501	2.79	0.433	4.55	0.352	6.28	0.273	10.4	0.264
2.03	4.86	0.132	1.92	0.0893	0.954	0.233	0.728	0.828	0.700	2.07	0.640	4.07	0.547	6.39	0.440	8.59	0.342	14.2	0.306
		0.297	2.45	0.157	1.17	0.411	0.938	1.36	0.892	3.23	0.803	5.99	0.673	8.89	0.540	11.8	0.408	17.7	0.363
		0.604	3.04	0.312	1.48	0.651	1.14	2.03	1.07	4.53	0.955	7.97	0.794	11.7	0.626	15.0	0.478	23.5	0.422
		1.63	3.84	0.637	1.90	1.24	1.44	3.17	1.34	6.92	1.16	11.4	0.957	16.0	0.745	20.0	0.569	31.1	0.506
		6.28	4.64	1.39	2.40	2.49	1.81	5.77	1.65	10.8	1.41	16.6	1.14	22.2	0.890	27.1	0.672	39.9	0.645
				2.67	2.94	4.17	2.26	9.37	2.01	16.2	1.69	23.1	1.37	29.7	1.07	35.3	0.835	52.2	0.694
				6.21	3.61	7.47	2.70	14.5	2.36	23.3	1.96	31.7	1.57	39.1	1.25	45.9	0.956	67.8	0.828
				14.8	4.22	14.2	3.22	23.5	2.77	34.3	2.27	43.8	1.85	52.9	1.45	61.7	1.07	87.9	0.971
				28.3	4.55	25.6	3.70	36.8	3.18	48.8	2.63	61.2	2.08	71.9	1.62	81.5	1.22	108	1.08
						40.0	4.00	52.7	3.41	66.1	2.82	79.2	2.24	90.5	1.77	101	1.35		

[a] *p* (kPa) and *n* (mol·kg^{-1}).

Table 2. Adsorption Equilibria of Pure H_2O on Zeolite 5A Using the Volumetric Method

0 °C		25 °C		50 °C		75 °C		100 °C	
p kPa	*n* mol·kg^{-1}	*p* kPa	*n* mol·kg^{-1}	*p* kPa	*n* mol·kg^{-1}	*p* kPa	*n* mol·kg^{-1}	*p* kPa	*n* mol·kg^{-1}
0.0493	10.9	0.0147	7.44	0.0267	5.11	0.0240	3.21	0.0480	2.62
0.171	12.4	0.036	8.61	0.0453	6.27	0.119	5.10	0.115	3.21
0.293	13.8	0.107	9.77	0.0760	7.44	0.212	6.26	0.461	5.09
		0.269	10.9	0.167	8.60	0.372	7.42	0.761	6.24
		0.833	12.4	0.423	9.76	0.739	8.57	1.27	7.38
		1.58	13.8	1.23	10.9	1.66	9.70		

Table 3. Adsorption Equilibria of Pure CO_2 on Zeolite 13X Using the Volumetric Method[a]

−45 °C		−25 °C		0 °C		25 °C		50 °C		75 °C		100 °C		125 °C		150 °C		175 °C	
p	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*	*p*	*n*
0.208	3.60	0.180	1.95	0.0982	0.844	0.0675	0.407	0.210	0.400	0.230	0.261	0.496	0.249	0.907	0.224	1.49	0.192	2.08	0.161
0.432	4.27	0.361	2.62	0.283	1.25	0.159	0.566	0.482	0.547	0.582	0.378	1.22	0.342	2.06	0.296	2.98	0.247	3.76	0.206
1.20	4.91	0.450	2.89	0.776	1.91	0.428	0.824	1.26	0.776	1.22	0.505	2.25	0.448	3.43	0.383	4.64	0.319	5.81	0.257
		1.06	3.54	1.83	2.53	1.07	1.20	2.82	1.10	2.79	0.689	4.61	0.588	6.41	0.491	8.09	0.402	9.68	0.320
		2.13	4.16	4.49	3.33	2.79	1.79	6.39	1.58	5.62	0.944	8.58	0.780	11.2	0.640	13.3	0.533		
		9.37	5.09	7.28	3.85	5.57	2.31	11.6	1.97	11.5	1.30	16.44	1.02	20.8	0.791	22.7	0.700		
				19.1	4.51	11.1	2.95	19.7	2.45	18.3	1.59	25.8	1.19						
						16.3	3.32	42.5	3.18										
						30.5	3.85												

[a] *P* (kPa) and *n* (mol·kg^{-1}).

Table 4. Adsorption Equilibria of Pure H_2O on Zeolite 13X Using the Volumetric Method

0 °C		25 °C		50 °C		75 °C		100 °C	
p kPa	*n* mol·kg^{-1}	*p* kPa	*n* mol·kg^{-1}	*p* kPa	*n* mol·kg^{-1}	*p* kPa	*n* mol·kg^{-1}	*p* kPa	*n* mol·kg^{-1}
0.0105	10.2	0.0035	6.25	0.0035	2.68	0.0119	2.68	0.0477	2.68
0.0686	12.1	0.015	8.40	0.0138	4.65	0.052	4.64	0.214	4.63
0.379	14.3	0.044	10.18	0.0278	6.25	0.122	6.25	0.487	6.23
		0.413	12.1	0.074	8.39	0.409	8.37	1.419	8.32
		1.83	14.2	0.085	8.57	0.443	8.55	1.52	8.49
				0.28	10.2	1.02	10.1		
				1.68	12.1				

Another isotherm model, the Sips model (i.e., the Langmuir−Freundlich model), has also been considered. The Sips model cannot describe all of the isotherms well with the same number of parameters used in the Toth model. Also, it does not have thermodynamically correct behavior (i.e., a proper Henry's law limit) as pressure approaches zero. Thus, isotherm results are shown only for the Toth model.

Water isotherms on silica gel have been measured at various experimental conditions with different silica gel sources. Bulck[5] adopted a Dubinin−Astakhov (D−A) equation to correlate the isotherm data from nine papers which presented original experimental adsorption data. Among these papers, only one result reported by Fraioli[12] used the same Davison grade 40 silica gel as we have to measure water vapor adsorption at 20 °C and relative pressures (p/p_0) between 0 to 1. We have compared Fraioli's data with ours, with the results shown in Figure 8. Fraioli's data at 20 °C lie slightly above our data at 25 °C and have a similar trend. We also tried the D−A model to describe water data on silica gel and obtained comparable results from Bulck's simulation.[5] However, the fitting result is not as good as with the Toth model and thus is not included in this paper.

Lee et al.[3] and Kim et al.[4] measured pure CO_2 and H_2O isotherms at (0 to 80) °C on zeolite 13X with a static volumetric method. The experimental data were correlated individually by the Toth model for each temperature. The saturation loading n_s for CO_2 varied from (9.01 to 6.44) mol·kg^{-1} and that for H_2O varied from (11.66 to 7.78) mol·kg^{-1} as temperature increases. We have obtained the monolayer saturation loading of 13.3 mol·kg^{-1} and 15.1 mol·kg^{-1} for CO_2 and H_2O, respectively.

Rege et al.[1] used a Micromeritics ASAP 2010 instrument and a Cahn TG-121 thermogravimetric analyzer to measure both pure CO_2 and H_2O isotherms at (22 and 70) °C on microporous

Table 5. Adsorption Equilibria of Pure CO_2 on Zeolites at 25 °C Using the Gravimetric Method

zeolite 5A		zeolite 13X	
p/kPa	n/mol·kg^{-1}	p/kPa	n/mol·kg^{-1}
0.00533	0.103	0.116	0.470
0.0147	0.169	0.237	0.676
0.0627	0.374	0.368	0.848
0.139	0.561	0.792	1.16
0.391	0.867	2.54	1.60
0.851	1.15	4.06	2.11
1.25	1.32	11.6	2.98
4.14	2.13	17.5	3.35
8.96	2.73	27.7	3.71
16.4	3.20	41.7	4.02
28.1	3.61	60.8	4.27
42.5	3.91	80.3	4.45
58.9	4.13		
73.1	4.27		
91.1	4.40		

Table 6. Adsorption Equilibria of Pure H_2O on Silica Gel Using the Volumetric Method

0 °C		25 °C		50 °C		75 °C	
p kPa	n mol·kg^{-1}	p kPa	n mol·kg^{-1}	p kPa	n mol·kg^{-1}	p kPa	n mol·kg^{-1}
0.0200	2.078	0.0271	0.980	0.0297	0.432	0.0139	0.107
0.0933	5.329	0.0889	2.07	0.115	0.977	0.113	0.427
0.200	10.5	0.408	5.31	0.363	2.06	0.466	0.957
0.368	15.6	0.941	10.4	1.88	5.25	1.50	2.00
0.540	19.0	1.60	15.5				
		2.43	18.9				

Table 7. Adsorption Equilibria of Pure CO_2 on Silica Gel Using the Gravimetric Method

10 °C		25 °C		40 °C		55 °C	
p kPa	n mol·kg^{-1}	p kPa	n mol·kg^{-1}	p kPa	n mol·kg^{-1}	p kPa	n mol·kg^{-1}
0.0672	0.00210	0.200	0.00437	0.0819	0.00120	0.131	0.00124
0.215	0.00609	0.445	0.00791	0.204	0.00267	0.373	0.00302
0.443	0.0117	1.000	0.0158	0.409	0.00487	1.03	0.00784
0.997	0.0272	2.83	0.0467	1.08	0.0122	2.89	0.0206
2.60	0.0731	9.79	0.152	3.31	0.0353	8.95	0.0598
10.6	0.263	16.8	0.245	11.1	0.112	17.3	0.110
22.1	0.477	25.9	0.353	20.1	0.191	29.6	0.182
41.6	0.775	39.9	0.505	36.4	0.320	45.2	0.266
62.1	1.03	60.7	0.699	57.9	0.468	63.4	0.357
85.7	1.28	77.4	0.841	83.4	0.630	87.1	0.478
		97.9	1.00				

Table 8. Toth Equation Parameters for Different Systems

system	a_0 mol·kg^{-1}·kPa^{-1}	b_0 kPa^{-1}	E K	t_0	c K
CO_2/5A	$9.875 \cdot 10^{-7}$	$6.761 \cdot 10^{-8}$	$5.625 \cdot 10^{3}$	$2.700 \cdot 10^{-1}$	$-2.002 \cdot 10^{1}$
H_2O/5A	$1.106 \cdot 10^{-8}$	$4.714 \cdot 10^{-10}$	$9.955 \cdot 10^{3}$	$3.548 \cdot 10^{-1}$	$-5.114 \cdot 10^{1}$
CO_2/13X	$6.509 \cdot 10^{-3}$	$4.884 \cdot 10^{-4}$	$2.991 \cdot 10^{3}$	$7.487 \cdot 10^{-2}$	$3.805 \cdot 10^{1}$
H_2O/13X	$3.634 \cdot 10^{-6}$	$2.408 \cdot 10^{-7}$	$6.852 \cdot 10^{3}$	$3.974 \cdot 10^{-1}$	-4.199
CO_2/SG	$7.678 \cdot 10^{-6}$	$5.164 \cdot 10^{-7}$	$2.330 \cdot 10^{3}$	$-3.053 \cdot 10^{-1}$	$2.386 \cdot 10^{2}$
H_2O/SG	$1.767 \cdot 10^{2}$	$2.787 \cdot 10^{-5}$	$1.093 \cdot 10^{3}$	$-1.190 \cdot 10^{-3}$	$2.213 \cdot 10^{1}$

adsorbents, including Linde 13X zeolite supplied as a binderless powder, activated γ-Al_2O_3, and three nonconventional adsorbents. Isotherm models such as the Sips, Toth, and the D−A equation were used to describe the data, and the D−A equation gave the best fit in the low-pressure range, particularly for water isotherms.

CO_2 isotherm data and model fits for comparable temperatures are shown in Figure 11. The isotherm from Kim et al.[4] is found to be slightly flatter and has a lower capacity than ours, whereas data from Rege et al.[1] have a steeper slope in the low concentration region and show higher capacity. The 13X sample that they used was in crystal form, unlike our sample with binder. This gives the higher capacity shown in Rege's work. The isotherm of Hyun and Danner[6] is close to our isotherm, being slightly lower in loadings. The sample they tested was from Linde (Union Carbide), and the different sample source may result in the small difference.

Conclusions

Equilibrium studies of pure CO_2 and H_2O on zeolites 5A and 13X and silica gel have been investigated experimentally by using volumetric and gravimetric apparatuses. Data have been obtained for CO_2 on zeolites 5A and 13X over the temperature range of (−45 to 175) °C and pressures up to 1 bar and for H_2O on zeolites 5A and 13X and silica gel at temperatures of (0 to 100) °C and pressures less than the saturation pressure at 25 °C. Isotherms for CO_2 on zeolites at room temperature were measured independently using two different techniques, and the results agree well with each other.

All of the isotherms have been described well by the multitemperature Toth equation, which uses only five parameters to describe the isotherms at different temperatures. Zeolites 5A and 13X show a great capacity to remove water vapor at low pressures, and silica gel has an increased relative capacity at high water pressures. Both zeolites give much higher CO_2 adsorption loadings than silica gel.

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