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Standard Isotherm Fit Information for Dry CO_2 on Sorbents for 4-Bed Molecular Sieve

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

LIST OF ACRONYMS AND SYMBOLS

4BMS	4-bed molecular sieve
CO_2	carbon dioxide
GRG	generalized reduced gradient

NOMENCLATURE

a	saturation capacity
a_0	saturation capacity at 0 K
$a_{0,j}$	constant for saturation capacity at 0 K on the j^{th} site
a_j	saturation capacity on the j^{th} site
b	affinity parameter
b_0	pre-exponential factor or adsorption entropy
$b_{0,j}$	constant for pre-exponential factor or adsorption entropy on the j^{th} site
b_j	affinity parameter on the j^{th} site
c_0	temperature dependence of the saturation capacity
$c_{0,j}$	constant for temperature dependence of the saturation capacity on the j^{th} site
E	adsorption energy
E_j	constant for adsorption energy on the j^{th} site
n	concentration of adsorbate
n_{meas}	measured amount adsorbed
n_{pred}	predicted amount adsorbed
p	adsorbate pressure
q_{st}	heat of adsorption
R	universal gas constant
T	absolute temperature

TECHNICAL MEMORANDUM

STANDARD ISOTHERM FIT INFORMATION FOR DRY CO_2 ON SORBENTS FOR 4-BED MOLECULAR SIEVE

1. INTRODUCTION

Onboard the International Space Station, one of the systems tasked with removal of metabolic carbon dioxide (CO_2) is a 4-bed molecular sieve (4BMS) system. In order to enable a 4-person mission to succeed, systems for removal of metabolic CO_2 must reliably operate for several years while minimizing power, mass, and volume requirements. This minimization can be achieved through system redesign and/or changes to the separation material(s). A material screening process has identified the most reliable sorbent materials for the next 4BMS. Sorbent characterization will provide the information necessary to guide system design by providing inputs for computer simulations.

The sorbent selected for removal of CO_2 is SYLOBEAD® MS S 544 Type 13X, referred to herein as Grade 544. The CO_2 adsorption properties as functions of temperature and pressure are characterized. Fitting of the resulting isotherms to an isotherm model are required to run computer simulations and develop an optimal system. This Technical Memorandum presents the selected model for fitting the data and the heat of adsorption results that can be extracted from the data fitting.

2. ISOTHERM MODELS

2.1 Langmuir Isotherm

In the general model,[1] the amount adsorbed, n, is given as:

$$n = \frac{abp}{1+bp} \ , \tag{1}$$

where

a = saturation capacity
b = affinity parameter
p = adsorbate pressure.

The saturation capacity and affinity parameter as functions of temperature are given, respectively, as:

$$a = a_0 + c_0/T \tag{2}$$

and

$$b = b_0 \times \exp\left(E/T\right) \ , \tag{3}$$

where

a_0 = saturation capacity at infinite temperature
c_0 = temperature dependence of the saturation capacity
b_0 = pre-exponential factor of the affinity parameter
E = adsorption energy
T = absolute temerature.

2.2 *k*-site Langmuir Isotherm

In the general model,[2] the amount adsorbed, n, is given as:

$$n = \sum_{j=1}^{k} \frac{a_j b_j p}{1+b_j p} \ , \tag{4}$$

where

a_j = saturation capacity on the j^{th} site
b_j = affinity parameter on the j^{th} site.

The saturation capacity and affinity parameter as functions of temperature are given as:

$$a_j = a_{0,j} + c_{0,j}/T \tag{5}$$

and

$$b_j = b_{0,j} \times \exp\left(E_j/T\right) , \tag{6}$$

respectively, where $a_{0,j}$, $c_{0,j}$, $b_{0,j}$, and E_j are constants for the j^{th} site analogous to their namesakes in the traditional Langmuir formulation.

3. FITTING METHODS

Two methods were used to find the empirically-determined fit parameters in equations 1–6. Both methods are implemented in Excel and use the Solver add-in which utilizes the generalized reduced gradient (GRG) nonlinear solver. The first method minimizes the sums of squares error:

$$\mathrm{SSE}=\sum\left(n_{\mathrm{pred}}-n_{\mathrm{meas}}\right)^2 , \tag{7}$$

where n_{meas} is the measured amount adsorbed and n_{pred} is the predicted amount adsorbed based on the isotherm model and fit parameters. The SSE is found by summing over all experimental measurements; thus, regions of measured data with higher pressures and lower temperatures which result in larger absolute values of n_{meas} and n_{pred} lead to higher absolute differences and are more emphasized in the resulting fit. The GRG nonlinear solver is converged to a residual of 1×10^{-12}. In order to help the solver converge, the parameters actively modified by the solver are normalized to be the same order of magnitude whereas the actual model parameters may be orders of magnitude different.

The second method minimizes the natural log of the SSE, which we will refer to as $\mathrm{SSE}_{\mathrm{log}}$:

$$\mathrm{SSE}_{\mathrm{log}}=\sum\left[\ln\left(\frac{n_{\mathrm{pred}}}{n_{\mathrm{meas}}}\right)\right]^2 . \tag{8}$$

Again, this is summed over all experimental measurements. Minimizing the $\mathrm{SSE}_{\mathrm{log}}$ results in a fit which emphasizes lower pressures than the first method as the relative proportion of error is minimized instead of absolute differences. This second method also uses the GRG nonlinear solver in Excel and a residual of 1×10^{-12} as the convergence criteria.

The product of this fitting process for isotherm data generated for Grade 544 Lot: 1000216159 is shown in figures 1 and 2. Figure 1 shows the results on a linear plot while figure 2 shows the results on a log-log plot. The data points measured for these plots are provided in table 1. The Langmuir model parameters used to generate the plots are given in table 2.

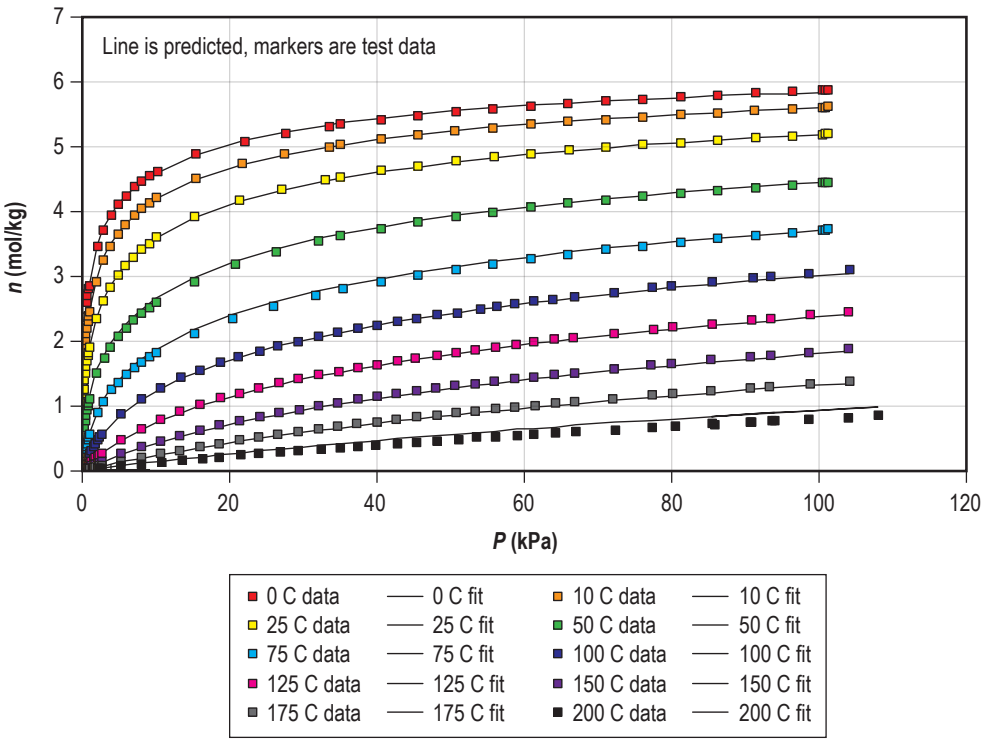

Figure 1. Grade 544 13X 3-site Langmuir fit CO_2 isotherms linear plot.

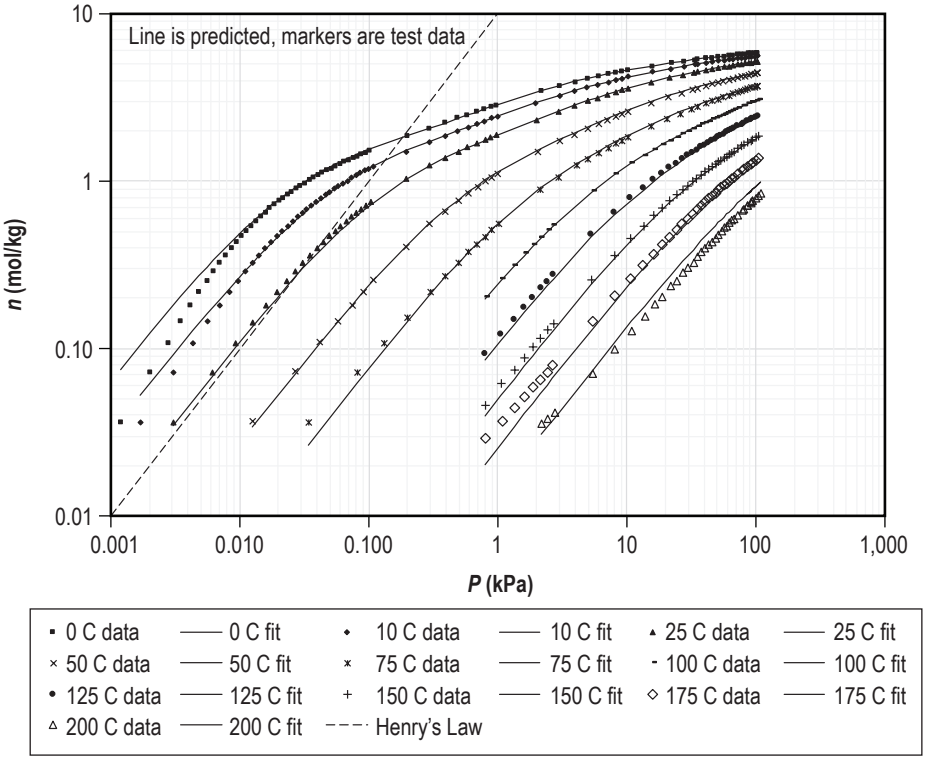

Figure 2. Grade 544 13X 3-site Langmuir fit CO_2 isotherms log-log plot.

Table 1. Data points measured for plots in figures 1 and 2.

0 C Data		10 C Data		25 C Data		50 C Data		75 C Data	
0 C		10 C		25 C		50 C		75 C	
P (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)
0.001193	0.036356	0.001703	0.036319	0.003049	0.036228	0.01267	0.036762	0.033835	0.036334
0.002039	0.072717	0.003072	0.072654	0.006087	0.072463	0.026859	0.073442	0.080701	0.072322
0.002791	0.109097	0.004341	0.108981	0.009173	0.108665	0.041786	0.11011	0.130698	0.108197
0.0035	0.14548	0.005632	0.145307	0.012425	0.144837	0.057481	0.146768	0.197858	0.153935
0.004183	0.181847	0.006919	0.18161	0.015798	0.180976	0.073813	0.183422	0.301711	0.219541
0.004871	0.218217	0.008228	0.217917	0.019301	0.217103	0.091052	0.220054	0.391976	0.272118
0.005572	0.254576	0.009579	0.254214	0.022977	0.253225	0.109007	0.256654	0.491256	0.326493
0.006291	0.290925	0.010975	0.290509	0.026835	0.289347	0.195294	0.409727	0.590988	0.377653
0.00704	0.327267	0.012478	0.326793	0.030867	0.32546	0.296283	0.555486	0.685978	0.422534
0.007819	0.363599	0.014043	0.363056	0.035132	0.361555	0.388072	0.664754	0.789294	0.468053
0.008636	0.399922	0.015691	0.399308	0.039587	0.397629	0.489297	0.766566	0.895381	0.512947
0.009427	0.436255	0.017434	0.435544	0.044353	0.433684	0.591976	0.85565	1.005872	0.557575
0.010283	0.472575	0.019288	0.471779	0.049417	0.469735	0.6925	0.930925	2.116892	0.890772
0.011262	0.508868	0.021239	0.508004	0.05477	0.505766	0.798786	1.002342	2.918522	1.059792
0.012313	0.545157	0.023304	0.54424	0.060384	0.541773	0.884728	1.053883	4.059185	1.246693
0.013426	0.581448	0.025519	0.580465	0.066396	0.577777	0.982738	1.108761	4.92112	1.360749
0.014602	0.617723	0.027862	0.616672	0.072604	0.61462	2.045019	1.514483	5.992976	1.483003
0.015862	0.654001	0.030278	0.652873	0.079322	0.651448	3.00088	1.745699	7.088253	1.590518
0.017173	0.690273	0.032964	0.689049	0.086613	0.688262	3.880945	1.910783	8.098809	1.678067
0.018596	0.726529	0.035845	0.725232	0.094437	0.725058	4.964935	2.075605	9.104698	1.757143
0.020029	0.762791	0.038913	0.761398	0.102845	0.761839	5.97544	2.206018	10.11308	1.829623
0.021658	0.799034	0.042208	0.797539	0.193889	1.048121	7.042308	2.324886	15.19822	2.122927
0.023426	0.835283	0.045726	0.833673	0.292963	1.247616	8.08972	2.427759	20.51016	2.354208
0.025324	0.871518	0.049511	0.869794	0.388172	1.391691	9.100981	2.517188	25.95266	2.543483
0.027363	0.907739	0.053579	0.905897	0.489418	1.511427	10.10752	2.599001	31.66621	2.708434
0.029473	0.943957	0.057895	0.941991	0.580828	1.602747	15.21455	2.924901	35.34615	2.80189
0.031882	0.980159	0.062662	0.978048	0.682273	1.690887	20.80487	3.183366	40.5599	2.919828
0.034485	1.01636	0.067794	1.014088	0.794183	1.77565	26.35163	3.38114	45.65861	3.022401
0.037298	1.052545	0.073315	1.050112	0.874912	1.832338	32.18311	3.547723	50.73232	3.113693
0.040344	1.088717	0.078967	1.086985	0.976941	1.897445	35.10962	3.620793	55.78334	3.198467
0.043546	1.124864	0.085248	1.123832	1.966476	2.33986	40.61392	3.740165	60.94186	3.275983
0.047131	1.160997	0.092087	1.160652	2.930904	2.622365	45.65392	3.836198	65.90539	3.345013
0.051014	1.197117	0.099635	1.197451	3.910625	2.838686	50.78231	3.921314	71.07226	3.411385
0.055105	1.233222	0.107761	1.234227	4.936354	3.019326	55.76423	3.996486	76.09665	3.472077
0.059642	1.269289	0.195871	1.516219	5.911591	3.162361	60.92672	4.066032	81.22372	3.528855
0.06453	1.305341	0.291254	1.719896	6.995504	3.297788	65.93164	4.127235	86.20155	3.583205
0.069779	1.341369	0.386323	1.875618	8.101616	3.416837	71.03564	4.184704	91.38735	3.634581
0.075422	1.377366	0.483119	2.003181	9.125581	3.513351	76.08841	4.237562	96.35121	3.682149
0.081203	1.414215	0.58166	2.113849	10.15035	3.599779	81.20635	4.286526	100.4261	3.71829
0.087579	1.451034	0.680557	2.20928	15.35638	3.929188	86.25184	4.331331	100.7957	3.725076

Table 1. Data points measured for plots in figures 1 and 2 (Continued).

0 C Data		10 C Data		25 C Data		50 C Data		75 C Data	
0 C		10 C		25 C		50 C		75 C	
P (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)
0.094519	1.48783	0.785822	2.299961	21.37716	4.181934	91.33274	4.373398	101.2066	3.732898
0.102071	1.524601	0.89748	2.386584	27.07755	4.354754	96.40446	4.413051		
0.197143	1.855308	0.980981	2.446268	33.05344	4.495367	100.4504	4.443011		
0.291375	2.074053	1.927877	2.924047	35.06401	4.536611	100.8098	4.448456		
0.386142	2.244574	2.974931	3.258044	40.61766	4.635793	101.1835	4.455331		
0.48859	2.391926	3.879466	3.467902	45.67714	4.713351				
0.578905	2.502513	4.885858	3.652103	50.77101	4.781936				
0.678632	2.604944	5.919544	3.803666	55.89908	4.842884				
0.775476	2.699147	7.080101	3.942701	60.93829	4.896974				
0.89789	2.802235	8.121851	4.048179	66.04166	4.946586				
0.974892	2.862821	9.156371	4.138539	71.05544	4.991007				
2.152862	3.46151	10.19449	4.218601	76.14763	5.032751				
2.994572	3.719335	15.48487	4.514646	81.2402	5.07124				
3.986878	3.941985	21.80498	4.740724	86.29507	5.106935				
4.940299	4.104323	27.41628	4.884113	91.38423	5.140505				
5.962473	4.243002	33.51694	5.005446	96.46283	5.172034				
7.198282	4.378216	35.05387	5.032928	100.488	5.195829				
8.13917	4.463775	40.65005	5.118906	100.8061	5.199708				
9.180574	4.545998	45.6707	5.185316	101.1903	5.204896				
10.23075	4.618584	50.6225	5.243239						
15.54642	4.883293	55.84894	5.297537						
22.16892	5.092234	60.92733	5.345289						
27.63659	5.216562	65.96554	5.388304						
33.50493	5.321477	71.02341	5.427946						
35.12723	5.347355	76.10714	5.464723						
40.68327	5.425095	81.18775	5.499072						
45.66445	5.485374	86.2888	5.531065						
50.76989	5.540069	91.31318	5.560438						
55.82067	5.588469	96.38674	5.588586						
60.8863	5.632383	100.4222	5.610054						
65.99825	5.673012	100.8097	5.614878						
71.0505	5.709872	101.2152	5.619267						
76.10918	5.743875								
81.21475	5.77562								
86.26366	5.805366								
91.34429	5.833146								
96.39878	5.859284								
100.4338	5.879303								
100.813	5.883632								
101.2182	5.887658								

Table 1. Data points measured for plots in figures 1 and 2 (Continued).

100 C Data		125 C Data		150 C Data		175 C Data		200 C Data	
100 C		125 C		150 C		175 C		200 C	
P (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)	*P* (kPa)	*n* (mol/kg)
0.796956	0.204192	0.796714	0.092563	0.793445	0.046325	0.797532	0.029173	2.185594	0.035959
1.062594	0.263446	1.057257	0.121171	1.065576	0.061835	1.077665	0.037054	2.436613	0.038334
1.32464	0.318886	1.330927	0.1487	1.329013	0.075423	1.34077	0.044429	2.743708	0.041632
1.594656	0.371979	1.601722	0.1756	1.593682	0.088896	1.606815	0.05176	5.364705	0.071655
1.869553	0.420806	1.864753	0.201953	1.858287	0.102303	1.868086	0.058731	8.02898	0.10015
2.126358	0.466903	2.155849	0.228318	2.128785	0.11575	2.124759	0.06553	10.89398	0.128806
2.407255	0.512802	2.414761	0.252106	2.406375	0.129391	2.39203	0.072483	13.66328	0.157542
2.659421	0.554048	2.664594	0.275442	2.678686	0.142594	2.659621	0.07943	16.32972	0.184908
5.373011	0.879958	5.335788	0.482236	5.333935	0.259298	5.349707	0.145259	18.60953	0.204912
7.996956	1.108299	8.030033	0.650988	8.005888	0.364556	8.008995	0.206839	21.60129	0.23722
10.64402	1.283864	10.5824	0.788908	10.60299	0.457067	10.59048	0.262748	23.96803	0.256429
13.42223	1.435504	13.32277	0.915158	13.32328	0.543443	13.2656	0.318098	26.83659	0.285846
15.93776	1.553519	16.03615	1.022129	15.97322	0.624248	15.95935	0.370382	29.33172	0.307492
18.75152	1.665194	18.76872	1.119921	18.70206	0.699093	18.60194	0.421109	32.42187	0.329811
21.24465	1.755456	21.33838	1.200756	21.4281	0.767338	21.29345	0.468796	35.08658	0.354209
24.10389	1.850068	24.00803	1.277457	24.09788	0.830433	24.00736	0.515278	37.53958	0.379335
26.62314	1.925302	26.693	1.350175	26.81313	0.891981	26.61368	0.558559	39.91645	0.39865
29.28653	1.999608	29.38812	1.418665	29.48744	0.947944	29.32639	0.602095	42.80288	0.424078
32.05443	2.068044	32.05043	1.482234	32.12829	1.00209	32.04043	0.641757	45.4316	0.436077
34.71755	2.13231	34.78754	1.538613	34.59849	1.047772	34.70835	0.680989	48.20017	0.461258
37.37826	2.193194	37.41199	1.596276	37.53251	1.100947	37.36213	0.718785	51.109	0.484058
40.05297	2.250978	39.97218	1.641781	39.96191	1.142452	40.00178	0.755267	53.5056	0.510117
42.90927	2.301525	42.81501	1.697049	42.60209	1.185956	42.67916	0.790715	56.21404	0.528687
45.46853	2.355962	45.25908	1.739992	45.33694	1.227863	45.44093	0.825101	59.15034	0.542973
48.23496	2.40297	48.17764	1.790112	48.05151	1.268649	48.10484	0.857469	61.25523	0.565821
50.89368	2.436943	50.73849	1.828623	50.6233	1.307692	50.75289	0.889649	64.17832	0.585887
54.03649	2.494131	53.28508	1.87076	53.31815	1.344179	53.39841	0.920065	67.08888	0.594404
56.23524	2.538178	56.21378	1.913616	56.03353	1.379245	56.07206	0.950409	72.37072	0.62869
58.73117	2.574498	58.87969	1.9526	58.70104	1.415736	58.75744	0.979977	77.40976	0.669896
61.33495	2.614375	61.25963	1.987413	61.34962	1.449654	61.46561	1.008135	80.47458	0.680521
63.96767	2.65194	63.9814	2.022875	64.06526	1.481165	64.17179	1.036163	85.80721	0.713296
66.82864	2.687034	66.73918	2.056147	66.77477	1.512333	66.84037	1.062605	90.78013	0.744086
72.15273	2.756907	72.11474	2.123251	72.18527	1.575234	72.00461	1.114461	93.5883	0.764552
77.45923	2.82282	77.5015	2.184802	77.27578	1.626754	77.36764	1.163738	98.70695	0.794646
80.01942	2.854725	80.06689	2.214289	79.98542	1.660142	80.08541	1.188788	103.9135	0.816857
85.49217	2.916153	85.56537	2.271688	85.26672	1.709473	85.32618	1.234496	108.1094	0.850145
90.97105	2.969399	90.8	2.327105	90.60868	1.758908	90.73334	1.276528	85.5699	0.723923
93.38592	2.99815	93.40138	2.353088	93.40792	1.784908	93.36245	1.30296	90.61602	0.758467
98.69335	3.047313	98.88293	2.40509	98.64322	1.828395	98.75441	1.343321	93.97134	0.771138
104.247	3.098333	103.992	2.451433	103.9757	1.876349	104.0956	1.383091		

Table 2. Langmuir model parameters used to generate plots in figures 1 and 2.

$b_{0,1}$	5.057×10^{-8}
E_1	5,584
$a_{0,1}$	1.640
$c_{0,1}$	8.350×10^{-9}
$b_{0,2}$	8.201×10^{-8}
E_2	4,408
$a_{0,2}$	2.537
$c_{0,2}$	1.417×10^{-8}
$b_{0,3}$	5.032×10^{-9}
E_3	4,408
$a_{0,3}$	1.995
$c_{0,3}$	-2.668×10^{-9}

4. ISOSTERIC HEATS OF ADSORPTION

The following information is paraphrased from reference 3:

The isosteric heat of adsorption, q_{st}, can be formulated in terms of measurable experimental variables using the Clausius-Clapeyron equation, expressed as:

$$q_{st} = RT^2 \left[\frac{\partial \ln(p)}{\partial T} \right]_n = -R \left[\frac{\partial \ln(p)}{\partial (1/T)} \right]_n \quad , \tag{9}$$

where

R = universal gas constant
p = adsorbate pressure
T = absolute temperature
n = adsorbed-phase concentration of adsorbate.

This equation assumes ideal gas behavior and that the adsorbed-phase volume is negligible. The subscript n indicates the amount adsorbed is held constant while evaluating the partial derivative, which necessarily makes $q_{st} = f(n)$. Since this method involves the derivative of a model, the original data used in the fitting operation must be of the greatest fidelity.

One method for determining isosteric heat of adsorption is to generate a plot of $\ln(P)$ versus $(1/T)$ at various determined loadings. Since loading is the independent variable and the equation is difficult to invert, the pressure is determined using equation solving tools in Excel. The resulting plot across loadings ranging from 0.05 to 5 mol/kg is shown in figure 3. The values used to generate this plot are provided in table 3. When the slope of each of the lines in figure 3 is multiplied by the ideal gas constant, the heat of adsorption is obtained which is shown in figure 4. The values used to generate this plot are provided in table 4.

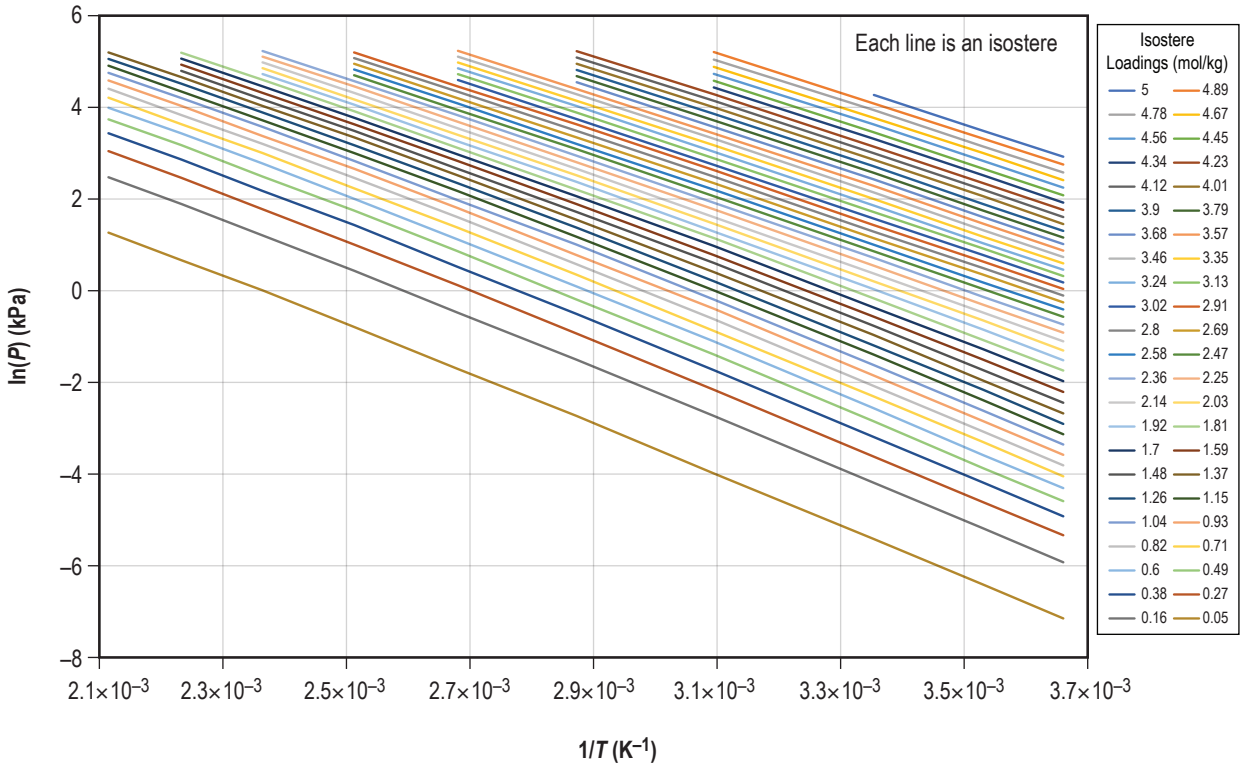

Figure 3. Plot of isosteres used to determine heat of adsorption for Grade 544 13X.

Table 3. Data used to generate plot in figure 3.

	ln(*P*)									
	1/*T*									
n	**3.66×10^{-3}**	**3.53×10^{-3}**	**3.35×10^{-3}**	**3.09×10^{-3}**	**2.87×10^{-3}**	**2.68×10^{-3}**	**2.51×10^{-3}**	**2.36×10^{-3}**	**2.23×10^{-3}**	**2.11×10^{-3}**
0.05	–7.15	–6.42	–5.42	–3.97	–2.74	–1.68	–0.78	–	0.68	1.28
0.16	–5.92	–5.19	–4.19	–2.74	–1.51	–0.46	0.44	1.22	1.90	2.49
0.27	–5.33	–4.60	–3.60	–2.15	–0.92	0.13	1.03	1.80	2.47	3.06
0.38	–4.92	–4.19	–3.18	–1.73	–0.50	0.54	1.43	2.20	2.87	3.45
0.49	–4.59	–3.85	–2.85	–1.40	–0.17	0.86	1.75	2.51	3.18	3.75
0.60	–4.30	–3.57	–2.56	–1.11	0.11	1.14	2.02	2.78	3.43	4.01
0.71	–4.05	–3.31	–2.30	–0.85	0.36	1.38	2.26	3.01	3.66	4.23
0.82	–3.81	–3.07	–2.06	–0.62	0.59	1.60	2.47	3.21	3.86	4.42
0.93	–3.58	–2.84	–1.83	–0.39	0.80	1.81	2.67	3.40	4.04	4.60
1.04	–3.35	–2.61	–1.61	–0.18	1.01	2.00	2.85	3.58	4.21	4.77
1.15	–3.13	–2.39	–1.39	0.03	1.20	2.18	3.02	3.75	4.37	4.93
1.26	–2.90	–2.17	–1.18	0.23	1.38	2.36	3.19	3.90	4.53	5.07
1.37	–2.67	–1.94	–0.96	0.42	1.56	2.53	3.35	4.05	4.67	5.21
1.48	–2.44	–1.72	–0.75	0.61	1.74	2.69	3.50	4.20	4.81	
1.59	–2.20	–1.49	–0.54	0.80	1.91	2.84	3.65	4.34	4.95	

Table 3. Data used to generate plot in figure 3 (Continued).

	ln(*P*)									
	1/*T*									
n	3.66×10^{-3}	3.53×10^{-3}	3.35×10^{-3}	3.09×10^{-3}	2.87×10^{-3}	2.68×10^{-3}	2.51×10^{-3}	2.36×10^{-3}	2.23×10^{-3}	2.11×10^{-3}
1.70	–1.97	–1.27	–0.34	0.97	2.07	2.99	3.79	4.48	5.08	
1.81	–1.74	–1.06	–0.15	1.15	2.23	3.14	3.93	4.61	5.21	
1.92	–1.51	–0.85	0.04	1.31	2.38	3.29	4.07	4.74		
2.03	–1.30	–0.65	0.22	1.47	2.53	3.43	4.20	4.87		
2.14	–1.10	–0.46	0.40	1.63	2.67	3.56	4.33	5.00		
2.25	–0.91	–0.29	0.56	1.78	2.82	3.70	4.46	5.12		
2.36	–0.73	–0.12	0.72	1.93	2.96	3.83	4.59	5.25		
2.47	–0.56	0.04	0.87	2.07	3.09	3.97	4.72			
2.58	–0.40	0.20	1.02	2.22	3.23	4.10	4.84			
2.69	–0.25	0.35	1.17	2.36	3.37	4.23	4.97			
2.80	–0.10	0.50	1.31	2.49	3.50	4.36	5.09			
2.91	0.05	0.64	1.45	2.63	3.63	4.48	5.21			
3.02	0.19	0.78	1.59	2.77	3.77	4.61				
3.13	0.33	0.92	1.73	2.91	3.90	4.74				
3.24	0.47	1.06	1.87	3.04	4.03	4.87				
3.35	0.61	1.20	2.01	3.18	4.16	5.00				
3.46	0.74	1.34	2.15	3.32	4.30	5.12				
3.57	0.88	1.48	2.29	3.46	4.43	5.25				
3.68	1.03	1.62	2.43	3.60	4.56					
3.79	1.17	1.77	2.58	3.74	4.70					
3.90	1.31	1.91	2.72	3.88	4.83					
4.01	1.46	2.06	2.87	4.02	4.97					
4.12	1.62	2.22	3.02	4.16	5.10					
4.23	1.77	2.37	3.17	4.30	5.24					
4.34	1.93	2.53	3.32	4.45						
4.45	2.09	2.69	3.48	4.60						
4.56	2.26	2.85	3.63	4.75						
4.67	2.42	3.01	3.79	4.90						
4.78	2.59	3.17	3.95	5.06						
4.89	2.77	3.34	4.12	5.22						
5.00	2.94	3.51	4.29							

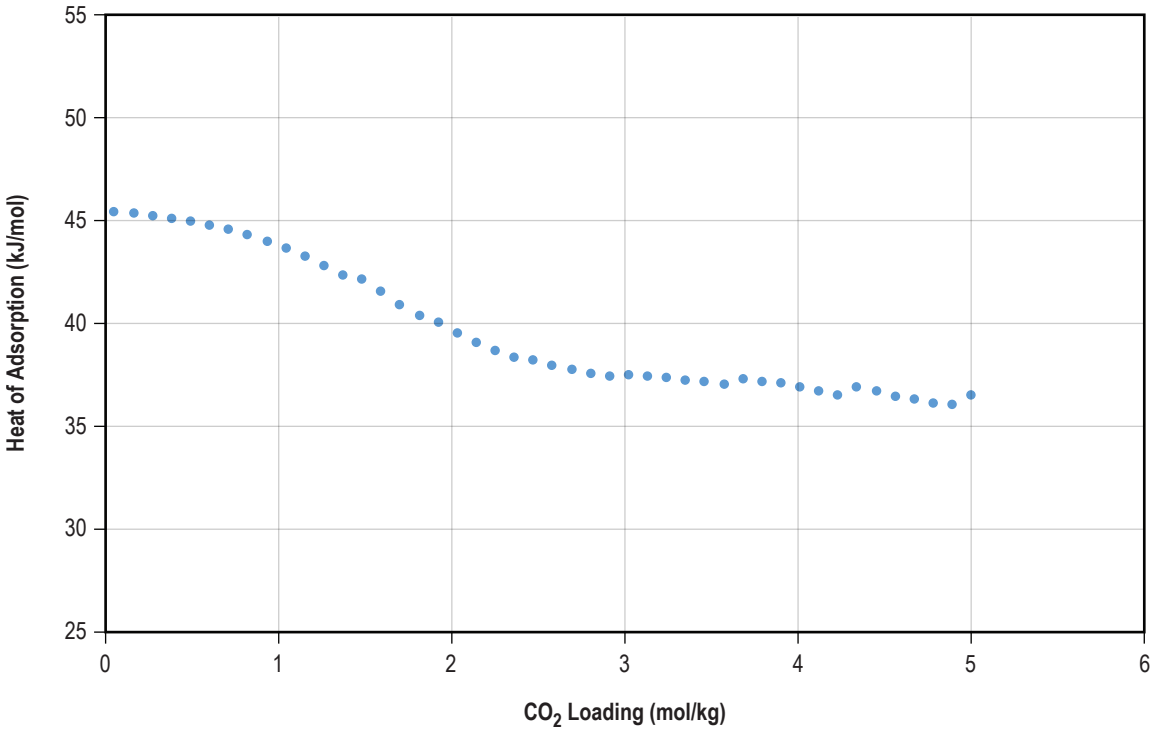

Figure 4. Heat of adsorption for CO_2 on Grade 544 13X.

Table 4. Data used to generate plot in figure 4.

n (mol/kg)	*Q* (kJ/mol)
0.05	45.4
0.16	45.4
0.27	45.3
0.38	45.1
0.49	45.0
0.6	44.8
0.71	44.6
0.82	44.3
0.93	44.0
1.04	43.7
1.15	43.3
1.26	42.8
1.37	42.3
1.48	42.1
1.59	41.6
1.7	41.0
1.81	40.4

Table 4. Data used to generate plot in figure 4 (Continued).

n (mol/kg)	*Q* (kJ/mol)
1.92	40.1
2.03	39.5
2.14	39.1
2.25	38.7
2.36	38.3
2.47	38.2
2.58	38.0
2.69	37.8
2.8	37.6
2.91	37.5
3.02	37.5
3.13	37.4
3.24	37.3
3.35	37.3
3.46	37.2
3.57	37.1
3.68	37.3
3.79	37.2
3.9	37.1
4.01	36.9
4.12	36.7
4.23	36.6
4.34	36.9
4.45	36.7
4.56	36.5
4.67	36.3
4.78	36.2
4.89	36.1
5	36.5

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14. ABSTRACT

Onboard the ISS, one of the systems tasked with removal of metabolic carbon dioxide (CO_2) is a 4-bed molecular sieve (4BMS) system. In order to enable a 4-person mission to succeed, systems for removal of metabolic CO_2 must reliably operate for several years while minimizing power, mass, and volume requirements. This minimization can be achieved through system redesign and/or changes to the separation material(s). A material screening process has identified the most reliable sorbent materials for the next 4BMS. Sorbent characterization will provide the information necessary to guide system design by providing inputs for computer simulations.

15. SUBJECT TERMS
4BMS, 4-bed molecular sieve, carbon dioxide, CO_2, adsorption, isotherm, zeolite

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