CO_2 Adsorption: Model Prediction and Alternative New Adsorbent

by

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Dissertation submitted in partial fulfillment
of the requirements for the
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Chemical Engineering

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CERTIFICATION OF APPROVAL

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Approved by:

Suriati Sufian

UNIVERSITI TEKNOLOGI PETRONAS
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January 2006

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

Sekibela Daisy Ntloana

ABSTRACT

The objective of this project is to determine the potential of CO_2 adsorption on pentace triptera leaves and a suitable model to describe its adsorption equilibrium relationship and to fit the adsorption data of CO_2 on molecular sieve 5A and on activated carbon using Langmuir and Sips model. Leaves were collected and cleaned. CHONS analysis was performed on the leaves. Data for adsorption of CO_2 on molecular sieve 5A and on activated carbon; AC1 was obtained from literature. Microsoft Excel and Polymath 5.1 software were used for data correlation.

The potential of CO_2 adsorption on pentace triptera leaves could not be determined due to equipment failure and therefore a model to describe its adsorption equilibrium relationship could not be deduced. Sips model showed a better fit for adsorption of CO_2 on both molecular sieve 5A and activated carbon at all temperatures studied.

ACKNOWLEDGEMENT

I would like to thank my supervisor; Mrs. Suriati Sufian for all the help she provided during the course of the project. Your patience and guidance is much appreciated.

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Data for CHONS analysis was provided by Mr Mohammed Zamri Abdullah. Thank you for kindly providing this information.

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NOMENCLATURE

q = Amount of adsorbate adsorbed, in mmol adsorbate/ g adsorbent
q_m = Equilibrium saturation capacity, in mmol/g
Q= Heat of adsorption, in KJ/ mol
T= Temperature, in K
K= Adsorption affinity constant, in KPa^{-1} or $Torr^{-1}$
c= Heterogeneity parameter for Sips parameter, unit less
P= Pressure, in KPa or Torr
R_g= Gas constant, in KJ/mol.K

CHAPTER 1

INTRODUCTION

1.1 Background

The development of new adsorbents for use of gas separation is rapidly gaining popularity. Various adsorbents have been used in the adsorption of CO_2. It is important to know the relationship between the adsorbent and adsorbate during the adsorption process. An important factor in choosing a suitable adsorbent is the adsorption equilibrium relationship data. The data is then used to model the adsorption process. Suitable adsorption isotherm models are used to describe the adsorption process of different adsorbate-adsorbent pairs.

1.2 Problem Statement

CO_2 is a primary green house gas. Emissions of CO_2 cause global warming. Strict environmental legislature has now been put in place to limit CO_2 emission to the atmosphere. One way to meet the environmental constraints is removing it from the process stream before discharging it to the atmosphere. One way to do so is by adsorption process. Suitable adsorbents must be used and the adsorbate-adsorbent relationship must be known to achieve separation effectively.

1.3 Objectives and Scope of Study

The objective of this project is to:

- To fit the adsorption equilibrium data to an adsorption isotherm model for activated carbon and molecular sieve 5A.
- To compare the performance of Sips and Langmuir models for the two adsorbents.
- To determine the potential of pentace triptera leaves as adsorbent for CO_2 and determine the model which will be suitable for modeling its adsorption data.

To meet the above mentioned objectives, analyses are performed on pentace triptera leaves to determine its composition. Experimental data on adsorption of carbon dioxide on activated carbon and molecular sieve is collected from literature [2, 5] and used for modeling purpose. The isotherm models used are Langmuir equation and Sips equation. The accuracy of the model is determined.

CHAPTER 2

THEORY

Adsorption is a process whereby a substance, known as an adsorbate, is accumulated on the surface of the solid, known as the adsorbent. The driving force for adsorption is unsaturated forces at the solid surface which can form bonds with the adsorbate. These forces are typically electrostatic or Van der Waals force.

There are two ways in which adsorption can occur; physical and chemical adsorption. Physical adsorption is characterized by van der Waals or electrostatic forces and the attraction depends on the polar nature of the adsorbate as well as that of the adsorbent.

Table 1.1: Comparisons between 2 types of adsorption

Physisorption **(Physical Adsorption)**	**Chemisorption** **(Chemical Adsorption)**
Low heat of adsorption (< 2 or 3 times latent heat of evaporation	High heat of adsorption (> 2 or 3 times latent heat of adsorption)
Monolayer of multilayer	Monolayer only
No dissociation of adsorbed species	May involve dissociation
Only significant at relatively low temperatures	Possible over a wide temperature range
Rapid, non-activated, reversible	May be slow, activated, irreversible
No electron transfer although polarization may occur	Electron transfer leading to bond formation between adsorbate and adsorbent

2.1 Adsorbents Used

Molecular sieve 5A and activated carbon were used in this study. Molecular sieve 5A used is manufactured by Union Carbide Co. It has total pore volume of $0.076 cm^3$, as determined by mercury displacement method. Its surface area as determined by BET method is $366 m^2/g$. It is mainly used in separation of the normal and isomerous alkenes; pressure swing adsorption for gases; co-adsorption of moisture and carbon dioxide.

Activated carbon used in this study is AC1. It has surface area of $3000 m^2/g$ and total pore volume of $1.6 cm^3/g$. It is most commonly used for separation of organic vapors from gases and decolorizing of aqueous solutions.

2.2 Adsorption Isotherms

The adsorption isotherm is the initial experimental step in an evaluation to determine feasibility of adsorption treatment and whether further test work should be conducted. It is a batch equilibrium test which provides data relating adsorbate adsorbed per unit weight of adsorbent to the amount of adsorbate remaining in solution.

During the process of adsorption dynamic phase equilibrium leads to a distribution of the solute between the fluid phase and the solid phase. The equilibrium is usually expressed in terms of:

1. Concentration (if the fluid is liquid) or partial pressure (if the fluid is a gas)of the adsorbate, and,
2. Solute loading on the adsorbent, expressed as mass, moles or volume of adsorbate per unit mass or pr unit area (determined as the BET monolayer-equivalent specific surface area) of the adsorbent.

2.2.1 Pure Gas Adsorption Isotherm Classification

IUPAC recently extended the original adsorption isotherm classification proposed by Brunauer, Deming, Deming and Teller to give six generic adsorption isotherms, as shown

in Figure 2.1.

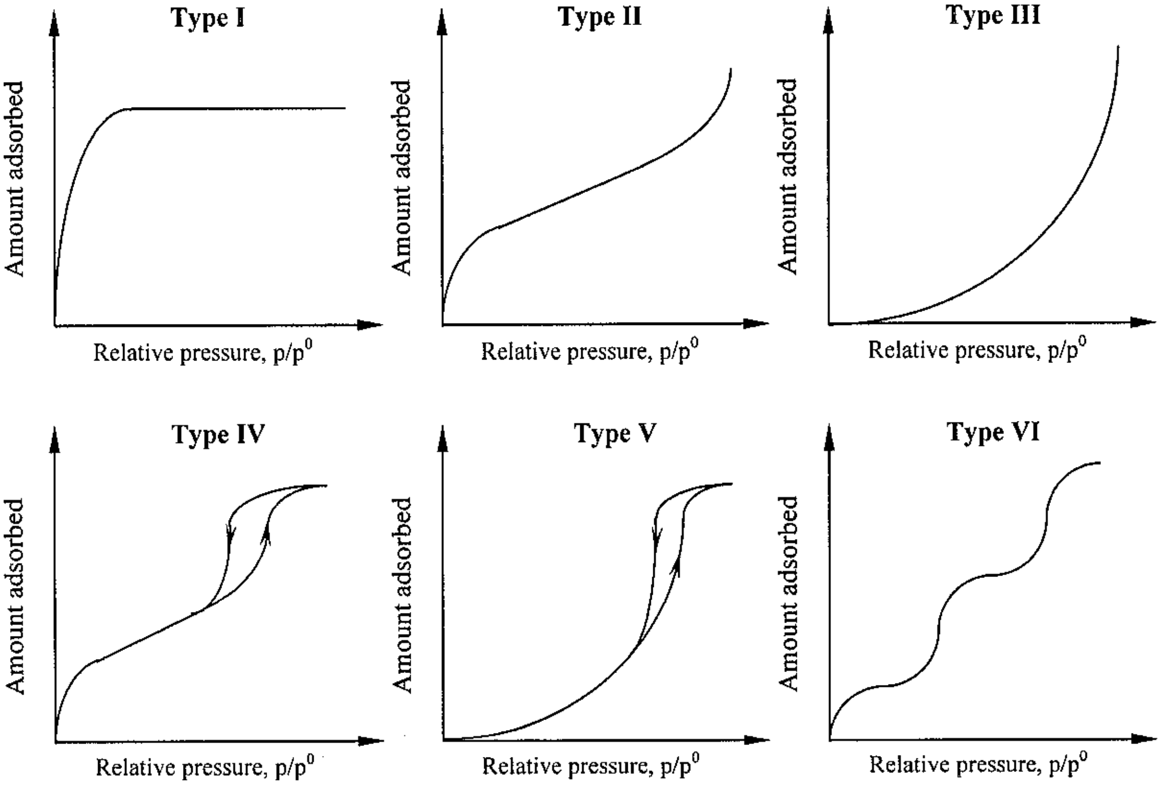


Figure 2.1: IUPAC classification of gas adsorption isotherms

2.2.2 Usefulness of Adsorption Isotherms

Inspection of adsorption isotherm provides the following useful information:

- Adsorbability of a component.
- The weight pick-up or the concentration of the adsorbate on the adsorbent.
- The degree of removal achievable as indicated by the equilibrium adsorbate concentration which remains unchanged with increasing adsorbate dosage.
- Sensitivity to adsorbate concentration change as indicated by relative steepness of the isotherm line.

2.2.3 Isotherm Models Used

- **Langmuir Isotherm**

The Langmuir isotherm model is based on the following assumptions:

- Surface is homogenous, meaning that adsorption energy is constant over all sites.
- Molecules are adsorbed at definite localized sites.
- Each site can accommodate only one molecule or atom.

The Langmuir isotherm is restricted to describing the classical Type I adsorption isotherm shape. The Langmuir equation is derived from a simple mass-action kinetics analysis.

Langmuir expression describing the amount adsorbed as a function of pressure:

$$q = \frac{q_m Kp}{1 + Kp} \qquad [1]$$

This isotherm expression may be rewritten as a linear expression to evaluate the equilibrium monolayer amount adsorbed, q_m, and the equilibrium constant for the adsorption and desorption processes, K.

The linear form of the isotherm is given as:

$$\frac{p}{q} = \frac{1}{Kq_m} + \frac{p}{q_m} \qquad [2]$$

Thus, a plot of P/q vs P will render the adsorption data as a straight-line graph with a slope of $1/q_m$ and an intercept of $1/Kq_m$. At low pressures for the condition where $KP \ll 1$, the Langmuir isotherm reduces to the Henry's Law expression. At high pressures, where $KP \gg 1$, the amount adsorbed asymptotically approaches q_m. For intermediate pressures, Eq. [1] is non-linear in pressure. In general, K will change with temperature whereas the value of q_m should remain reasonably constant since it defines a "constant" related to the specific surface area of the adsorbent.

The temperature dependence of the affinity constant K, is given as:

$$K = k\infty \exp\left(\frac{Q}{RT}\right) \qquad [3]$$

- **Sips Isotherm**

It describes monolayer adsorption on energetically heterogeneous solids. It is obtained by assuming that the surface is heterogeneous in the sense that the adsorption energy is distributed and that the sites having the same adsorption energy are grouped together. It is a special case of Langmuir isotherm. For energetically homogeneous solid it reduces to Langmuir isotherm. It may be also considered a monolayer modification of a simple Freundlich isotherm, which does not display monolayer behavior.

The equation for Sips isotherm is:

$$q = \frac{q_m(KP)^{(1/c)}}{1+(KP)^{(1/c)}} \qquad [4]$$

The affinity constant has the same temperature dependence relationship as the Langmuir equation.

2.3 Isosteric Heats of Adsorption

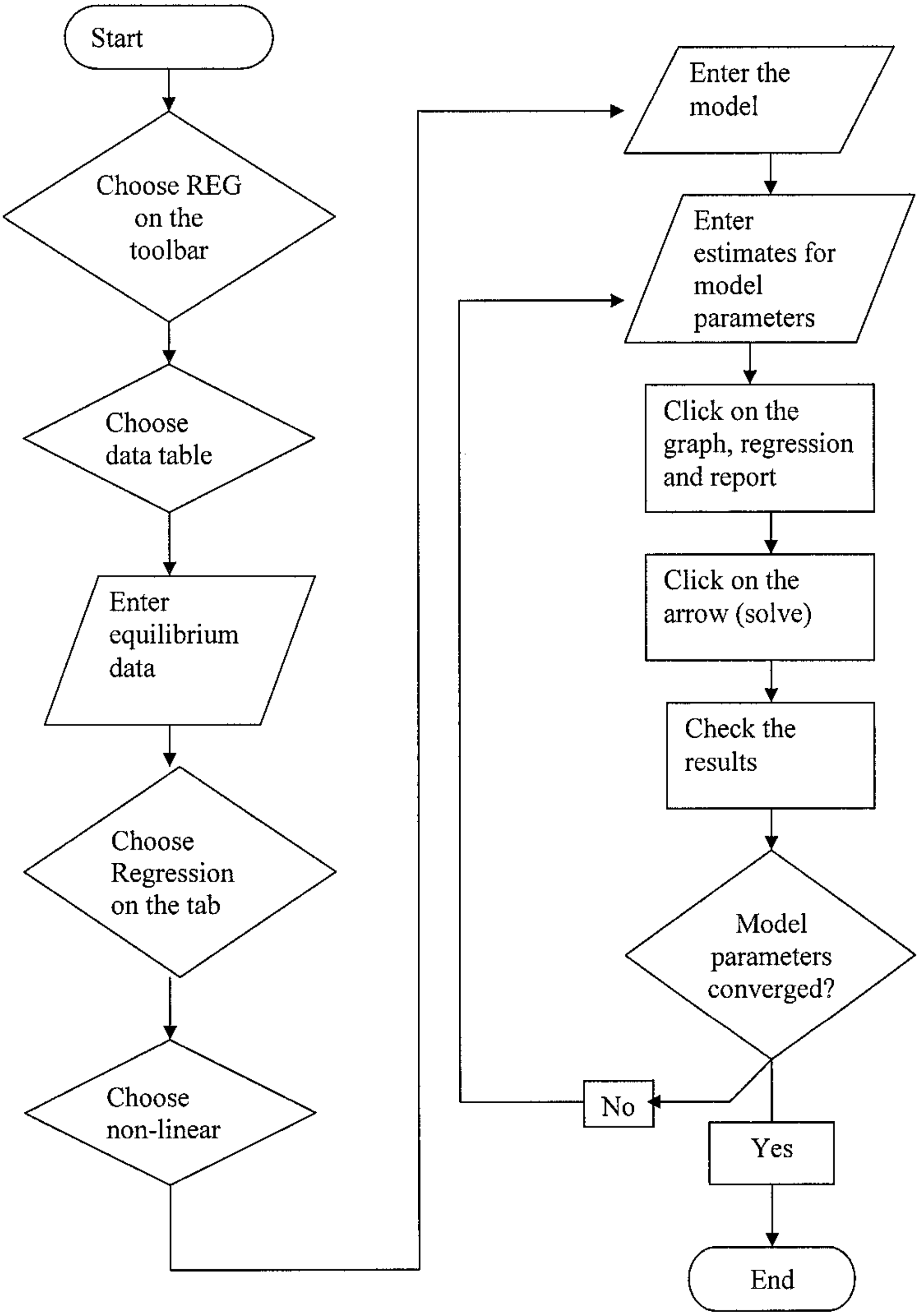
Physical adsorption process is always accompanied by a decrease in heat. Integral heat of adsorption is the total heat released when the adsorbate loading is increased from zero to a final value under isothermal conditions. As the heat of adsorption increases, the adsorbed amount increases due to the higher energy barrier that the adsorbed molecules have to overcome to evaporate back into gas phase. Increasing the temperature will decrease the amount adsorbed due to the greater energy acquired by the adsorbed molecules. The magnitude of the heat of adsorption can provide useful information about the nature of the surface and the adsorbed phase. Generally, an initial sharp decrease of heat of adsorption with increasing adsorbate loading reveals site heterogeneity whereas the flat heat profile with increasing adsorbate loading indicates a balance between strength of energetic heterogeneity of adsorbate-adsorbent interactions and adsorbate-adsorbate interactions.

Isosteric heat of adsorption can be calculated by applying the Claussuis-Clayperon equation,

$$Q = R_g\left(\frac{T_1T_2}{T_2-T_1}\right)\ln\left(\frac{P_2}{P_1}\right) \qquad [4]$$

This plain method is based on the assumption that the value of the isosteric heat of adsorption does not depend on temperature for a certain surface loading. To apply the method, only two sets of the experimental isotherm data at two different temperatures are needed. If Q is temperature independent, the graph of ln P against 1/T must result in a straight line, with Q as the slope of the graph.

3.4 Polymath Methodology



CHAPTER 4

RESULTS AND DISCUSSION

4.1 Adsorption of CO_2 on Molecular Sieve 5A

4.1.1 Adsorption isotherm

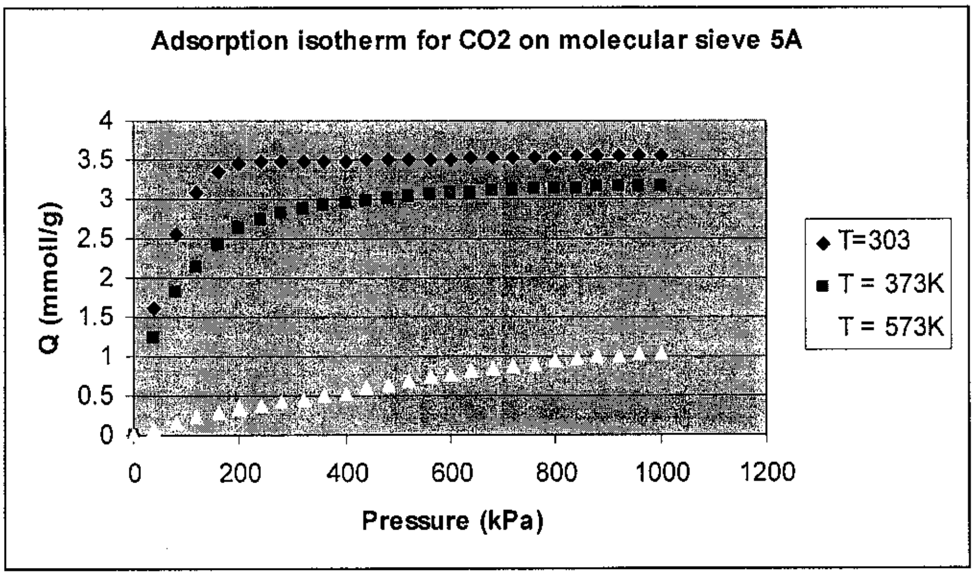


Figure 4.1: Adsorption isotherm of CO_2 on molecular sieve 5A

4.1.2 Langmuir fit to adsorption data

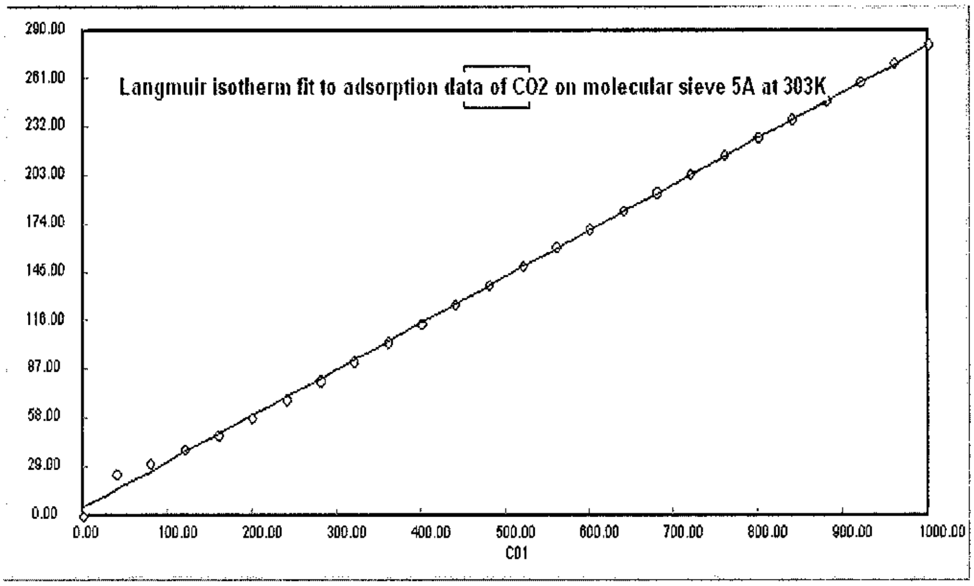


Figure 4.2: Plot of P/Q against P for Langmuir fit at 303K

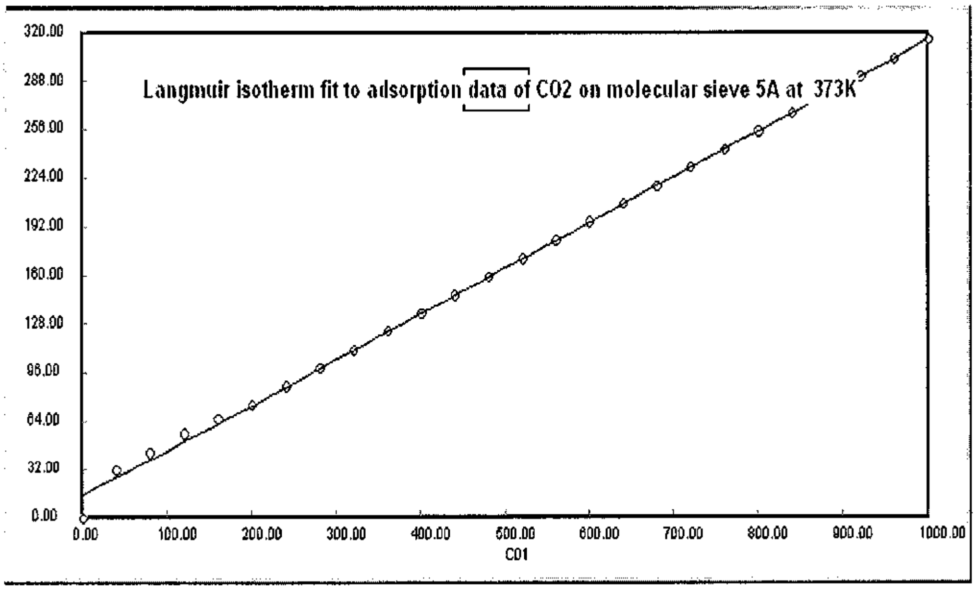


Figure 4.3: Plot of P/Q against P for Langmuir fit at 373K

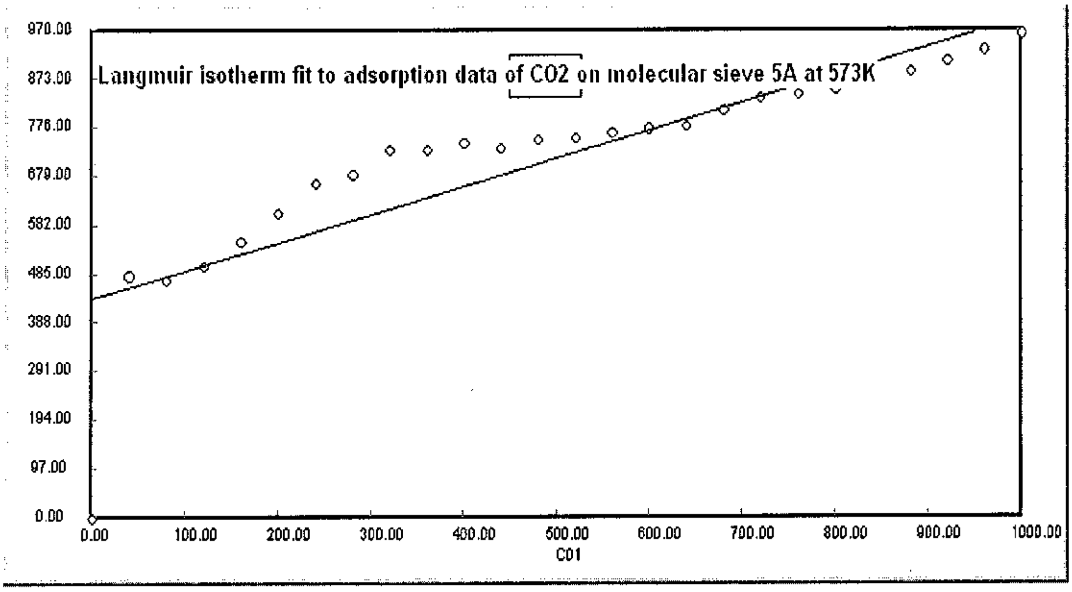


Figure 4.4: Plot of P/Q against P for Langmuir fit at 573K

Table 4.1: Parameters for Langmuir equation for molecular sieve 5A

Temperature (K)	Equation	q_m (mmol/g)	K (KPa^{-1})
303	Y= 0.2761x + 5.1057	4.817	0.04
373	Y = 0.3005x + 15.47	3.33	0.019
573	Y = 0.5583x + 437.55	1.791	1.27E-03

Equilibrium data for the adsorption of CO_2 was modeled with the two models: Langmuir and Sips model. Figure 4.1 shows the isotherm for the equilibrium data for molecular sieve 5A. Figures 4.2, 4.3 and 4.4 show the approximation using Langmuir isotherm. Langmuir isotherm resulted in a good fit for data for lower temperature adsorptions, i.e. 373K and 303K. At 573K, data showed a deviation from the isotherm behavior. This might be attributed to the fact that at high temperature, the adsorption heat increases. As it does so, thermal agitation of the adsorbed molecules increases. The adsorbed molecule will therefore have interactions with the adsorbate molecules immediately around it. Langmuir model representation does not take into account such interactions. At the same time, as the temperature is increased, the value of K; the affinity constant decreases. This is an indication of the decreased interaction between the adsorbate and adsorbent and hence the weakening of the bond between them. The value of the saturation capacity is not constant at all temperatures.

4.1.3 Sips Fit to Adsorption Data

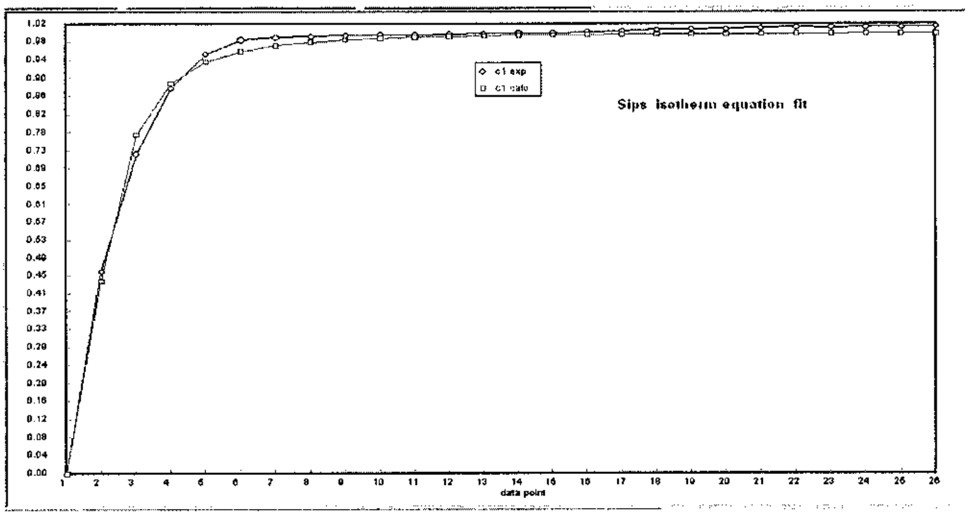


Figure 4.5: Sips fit to adsorption data of CO_2 on molecular sieve 5A at 303K

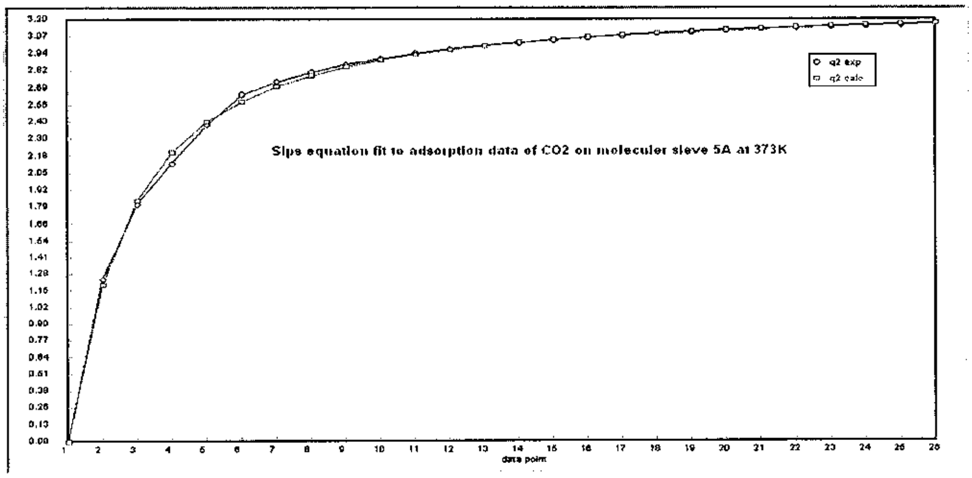


Figure 4.6: Sips fit to adsorption data of CO_2 on molecular sieve 5A at 373K

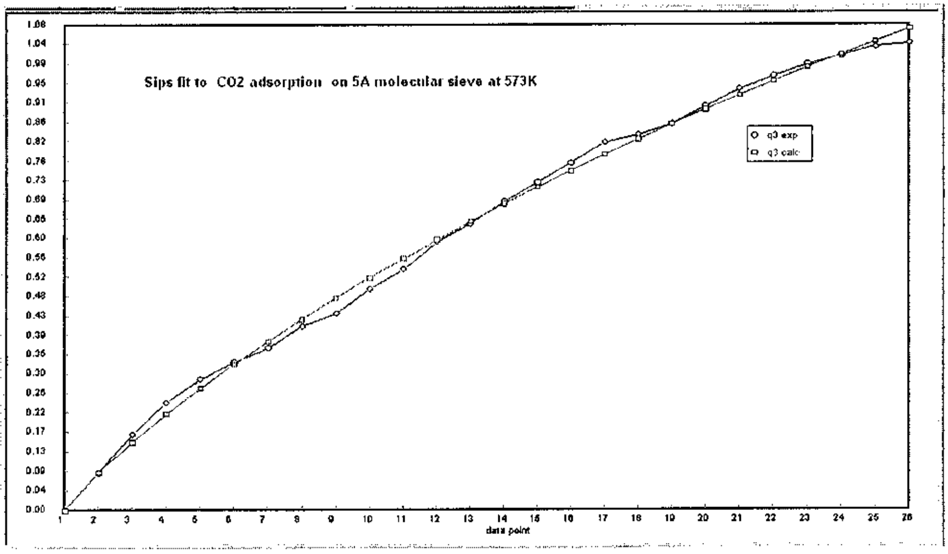


Figure 4.7: Sips fit to adsorption data of CO_2 on molecular sieve 5A at 573K

Table 4.2: Parameters for Sips equation for molecular sieve 5A

Temperature	**q_m (mmol/g)**	**K (KPa^{-1})**	**c**
303K	3.5534	0.02	0.5195
373K	3.3138	0.0151	0.894
573K	3.94395	3.26E0-4	1.13

Figures 4.5 to 4.7 show the approximation of data using Sips model at temperatures 303K, 373K and 573K respectively. Sips model shows a better fit to adsorption data than Langmuir model at all temperatures. This is because of the flexibility of the isotherm model as introduced by the inclusion of an additional parameter, c. This parameter gives an indication of the deviation of the isotherm model from the Langmuir behavior. For the data at 303K and 373K, this value is small, as expected. It shows that the deviation from the Langmuir behavior is small. Pronounced deviation is observed from data at 573K. The parameter c is greater than 1, showing a positive deviation from Langmuir behavior. The constant K has the same meaning in the Sips equation as it does in the Langmuir equation. The behavior it showed when Langmuir model was applied to data analysis still applies here. It decreases as the temperature increases.

Tables 4.1 and 4.2 shows the parameters for Langmuir and Sips parameters respectively. The values obtained for saturation capacity; q_m are different for the two models. Sips model shows higher values of equilibrium constant than Langmuir model. The values for saturation capacity are supposed to be independent of temperature. According to the results of our model, it is not the case. The difference in the three values is observed to be larger when Langmuir model is used. When Sips model is used, the difference in values is not that much: 3.553 mmol/g, 3.313 mmol/g and 3.94 mmol/g as opposed to 4.81mmol/g, 3.33 mmol/g and 1.791 mmol/g respectively. This also shows that Langmuir model is inadequate in describing adsorption data of molecular sieve 5A.

Table 4.3: Comparisons of error between Langmuir and Sips models

Model	**Standard deviation, R^2**		
	303K	**373K**	**573K**
Langmuir	0.992	0.999	0.74
Sips	0.998	0.999	0.997

Table 4.3 shows the R^2 values obtained when fitting Langmuir and Sips model. The values confirm that Sips model gives a better fit than Langmuir at all temperatures studied. However, the standard deviation value is the same for both models at 373K. At 573K, the R^2 value is the lowest, showing that the deviation from model assumption is the highest.

4.1.4 Isosteric Heats of Adsorption

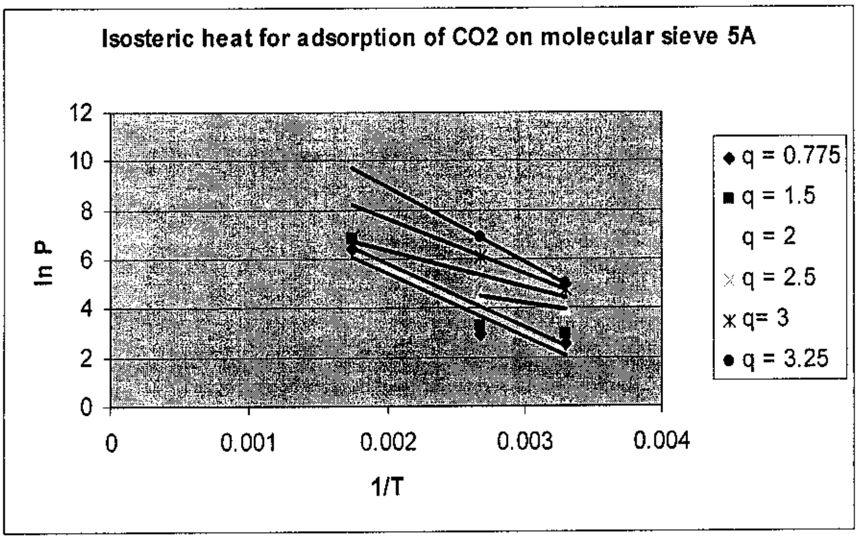


Figure 4.8: Isosteric heat of adsorption

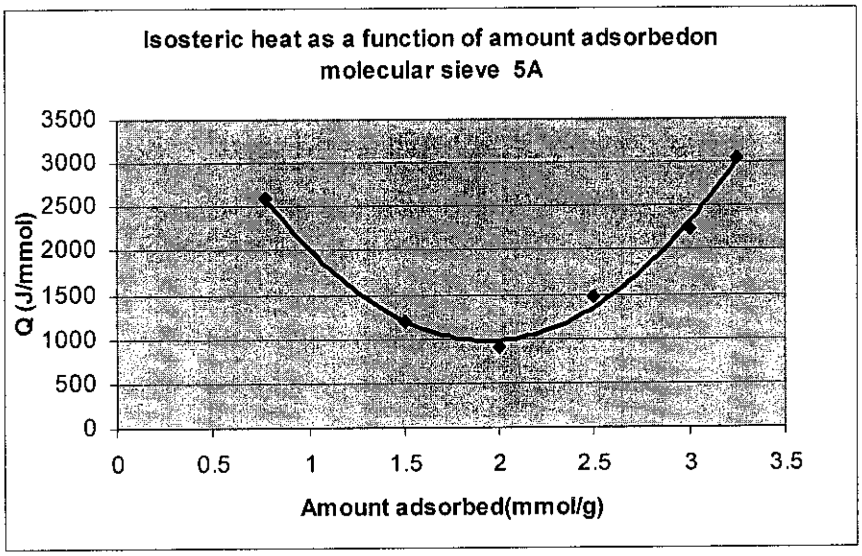


Figure 4.9: Isosteric heat variation with adsorbed amount

Figure 4.8 shows the adsorption isoster plot used to get heat of adsorption. The slope of the plot gives the heat of adsorption. The plot yields a straight line indicating that the heat of adsorption does not vary temperature. Figure 4.9 shows change of isosteric heat with the quantity of adsorbate adsorbed. As expected, the amount adsorbed increases with the increase in heat of adsorption. Initially, there is a decrease in Q. This is an indication that the surface is energetically heterogeneous. The adsorption energy is not distributed uniformly around the adsorptive sites, as Langmuir model assumes. The steepness of the plot indicates the degree of heterogeneity.

4.2 Adsorption of CO_2 on Activated Carbon

4.2.1 Adsorption isotherm

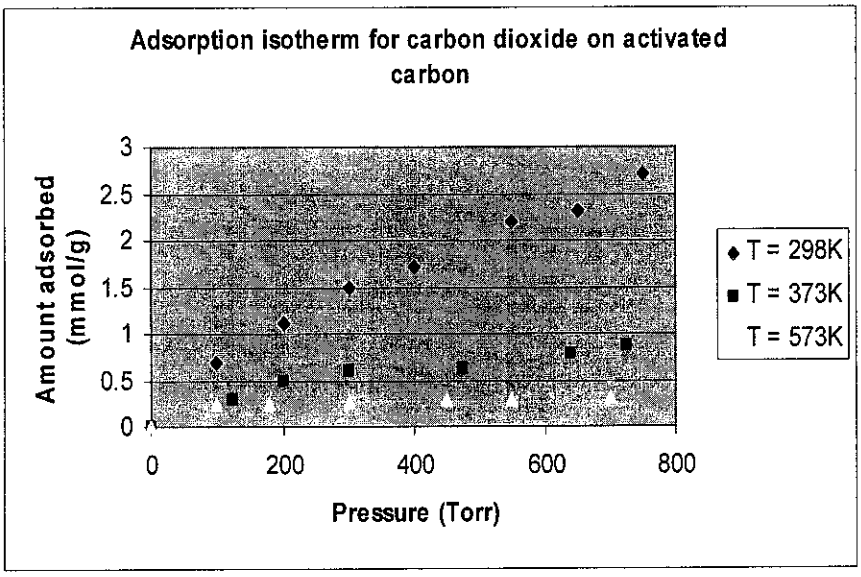


Figure 4.10: Adsorption isotherm for CO_2 on activated carbon

4.2.2 Langmuir fit to adsorption data

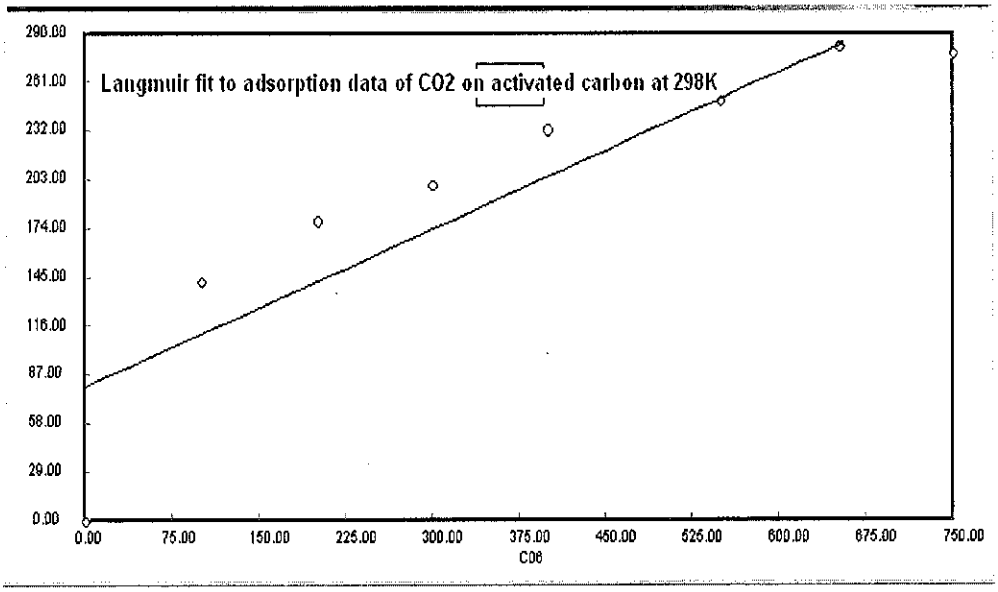


Figure 4.11: Plot of P/Q against P for Langmuir fit at 298K

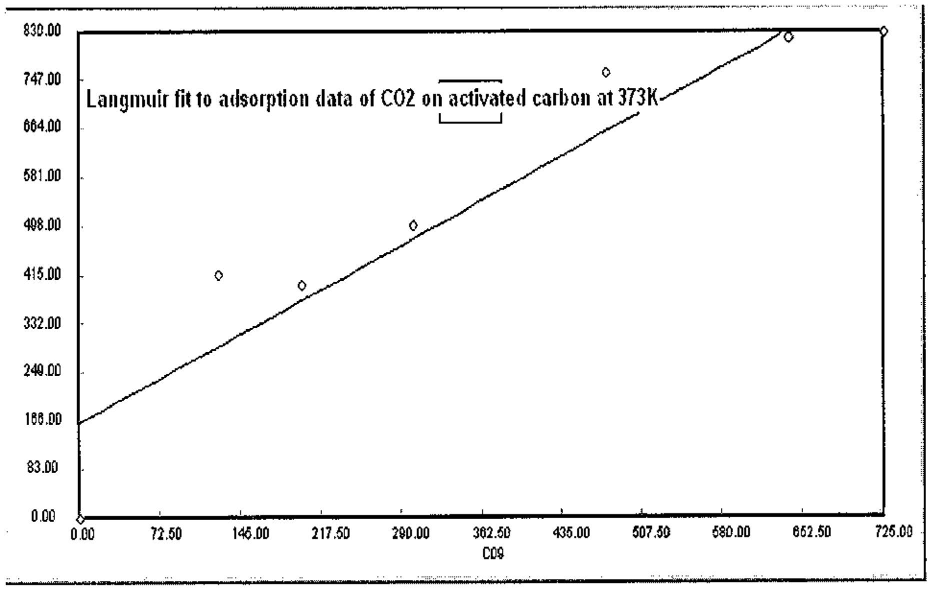


Figure 4.12: Plot of P/Q against P for Langmuir fit at 373K

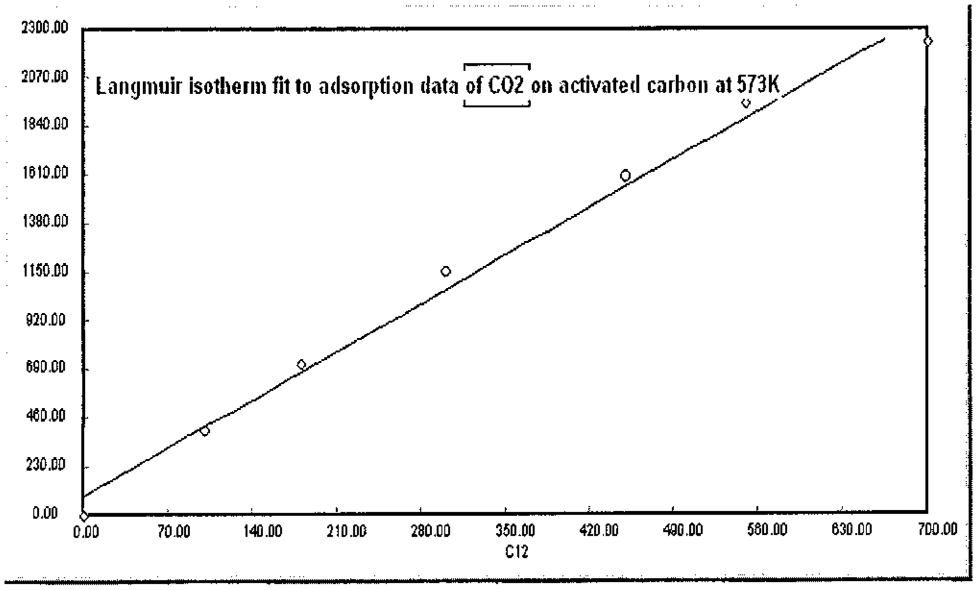


Figure 4.13: Plot of P/Q against P for Langmuir fit at 573K

Table 4.4: Parameters for Langmuir equation

Temperature (K)	Equation	q_m(mmol/g)	K(Torr^{-1})
298	Y = 0.311x + 80.74	3.125	4E-03
373	Y = 1.042x + 165.3	0.9597	6.3E-03
573	Y = 3.244x + 96.55	0.3086	0.034

The adsorption isotherm for adsorption of CO_2 on activated carbon is shown in Figure 4.10. The equilibrium data is approximated using Langmuir isotherm, shown in figure 4.11 to figure 4.13. Again, Langmuir isotherm does not fit data as well as Sips model does. Surprisingly, at high temperature of 573K, the fit is better as indicated by the standard deviation, R^2 of 0.9895. There is a big difference in the value of the saturation capacity as obtained using the two models. The values are not close. For Langmuir isotherm, they are as follows: 3.125 mmol/g, 0.9597 mmol/g and 0.3086 mmol/g for adsorption data at 303K, 373K and 573K respectively. Sips model is better in this regard than the Langmuir model: 0.406 mmol/g, 0.352 mmol/g and 1.601 mmol/g. This difference in values can be the result of experimental error as well as modeling error. The adsorption affinity constant; K, shows the expected behavior, it decreases as the temperature increases.

4.2.2 Sips fit to adsorption data

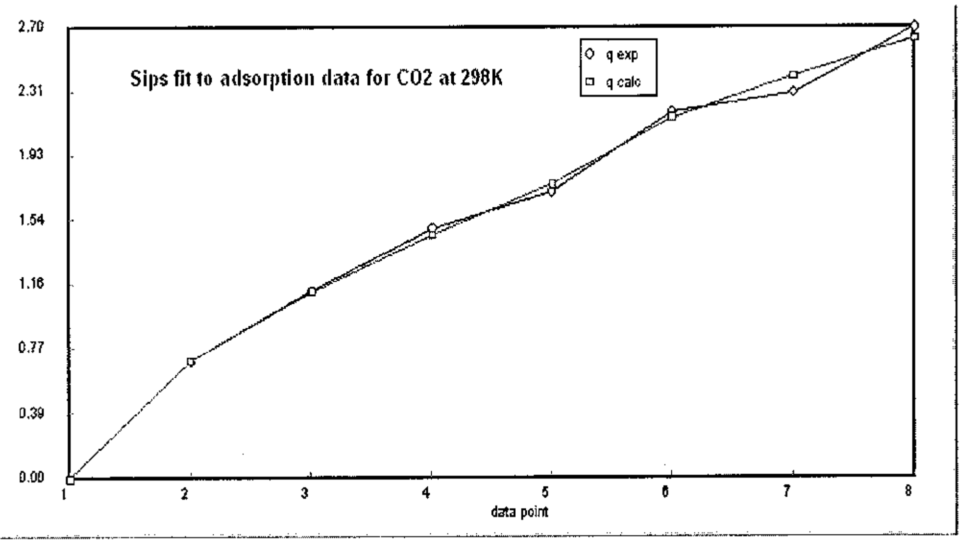


Figure 4.14: Sips fit to adsorption data of CO_2 on activated carbon at 298K

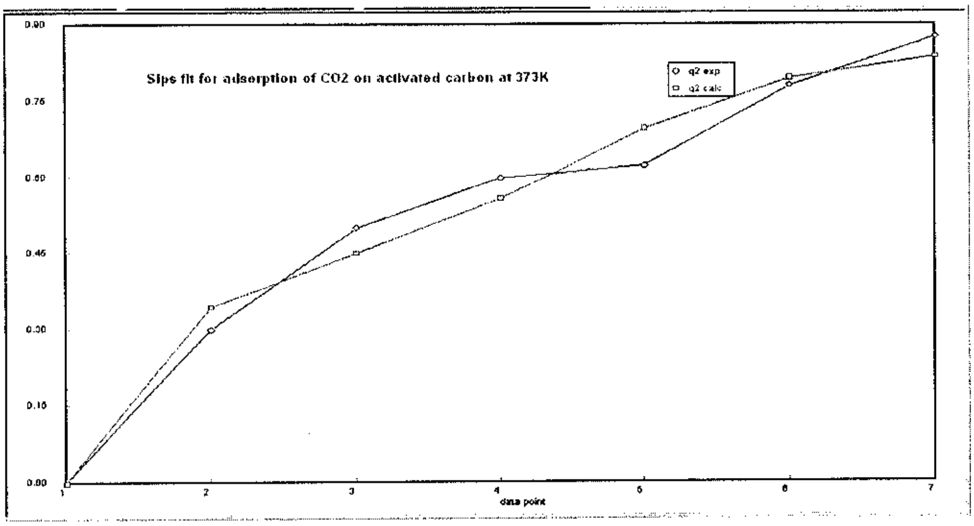


Figure 4.15: Sips fit to adsorption data of CO_2 on activated carbon at 373K

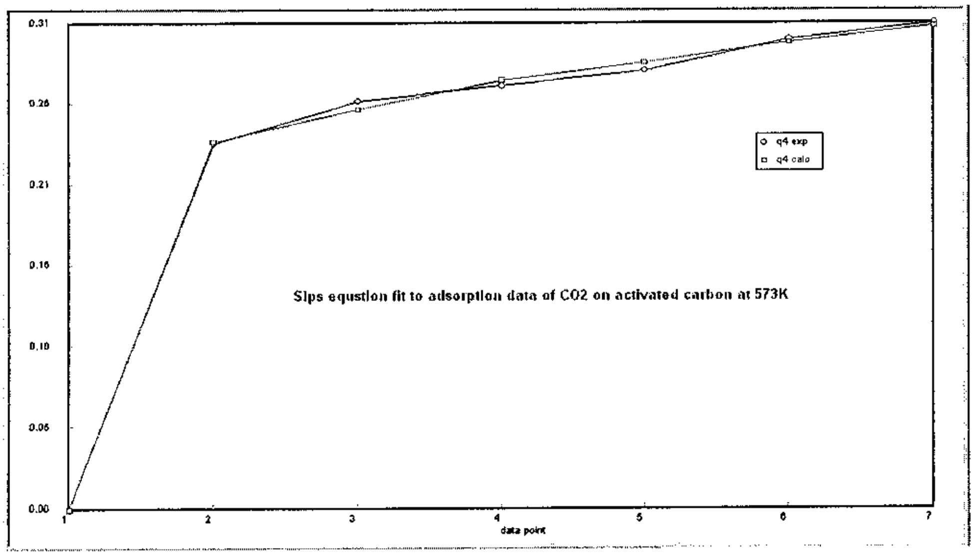


Figure 4.16: Sips fit to adsorption data of CO_2 on activated carbon at 573K

Table 4.5: Parameters for Sips equation

Temperature (K)	**q_m (mmol/g)**	**K($Torr^{-1}$)**	**c**
298	0.406	3.5E-03	1.54
373	0.352	5.3E-04	2.03
573	1.601	5E-10	7.074

Figures 4.14 to 4.16 shows Sips model fit to equilibrium data. Sips model fits the data better than the Langmuir model at all temperatures studied. Graphically, a good fit is shown and the modeling parameters agree well with theory except for saturation capacity which is not constant at all temperatures. The affinity constant decreases with increase in temperature and c increases with increase in temperature. The values of c, which are greater than 1 at all temperatures, show deviation from Langmuir model. It also shows that the adsorption energy of the adsorbent surface is heterogeneous.

Table 4.6: Comparisons of error between Langmuir and Sips models

Model	**Standard deviation, R^2**		
	298K	**373K**	**573K**
Langmuir	0.883	0.885	0.989
Sips	0.998	0.999	0.997

Table 4.6 shows the comparison of error for the two models. Sips model shows a better fit at all temperatures. Strangely, at 573K, Langmuir model fit the data better than at lower temperatures. The deviation from Langmuir behavior is expected to be the most at high temperature since the surface heterogeneity increases with temperature.

4.2.1 Isosteric Heats for CO_2 Adsorption on Activated Carbon

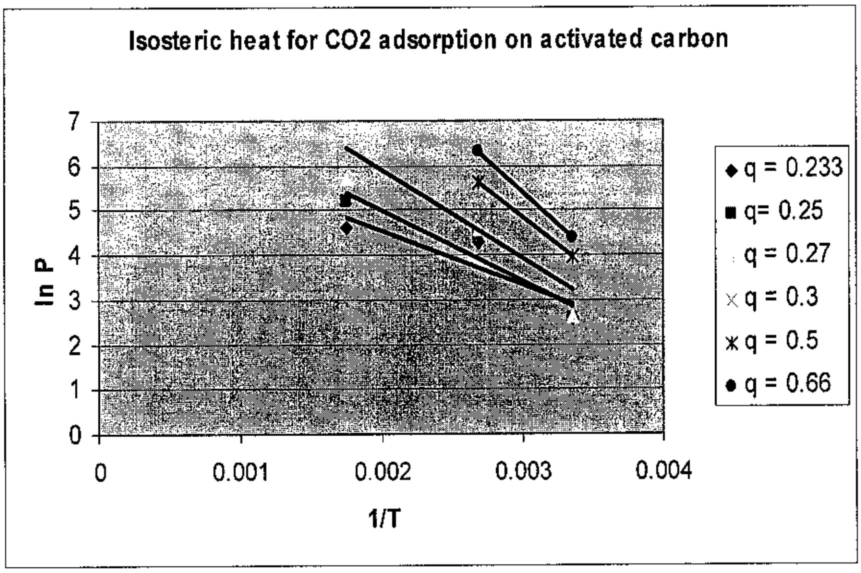


Figure 4.17: Graph of ln P vs. 1/T used to determine isosteric heats

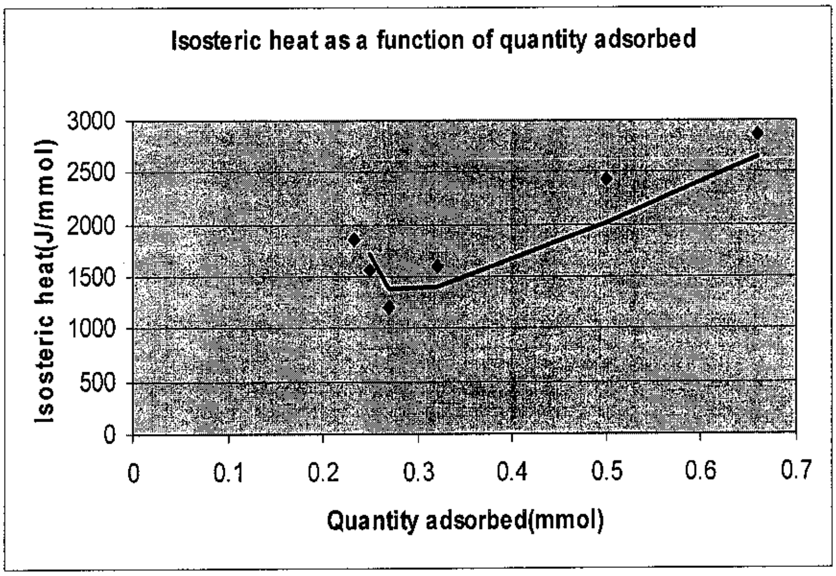


Figure 4.18: Isosteric heats variation with quantity adsorbed

Plots of adsorption isosters are shown in figure 4.17. Again, the plot of ln P against 1/T gives a straight line, indicating that the heat of adsorption is temperature independent. The plot of heat of adsorption against the amount adsorbed; figure 4.18 shows an initial decrease in Q, followed by a decrease as adsorption proceeds, i.e. as the amount adsorbed increases. The steepness is attributed to heterogeneity of the adsorptive sites of the adsorbent. Again, this shows as deviation in the Langmuir model.

4.3 Composition of Pentace triptera leaves

Table 4.7: CHONS analysis for Pentace triptera leaves

Constituent	**Carbon**	**Hydrogen**	**Oxygen**	**Nitrogen**	**Sulphur**
Percentage	46.35	6.73	43.77	2.8	0.33

Table 4.3 shows the composition of pentace triptera leaves. It can be seen that the leaf is rich in carbon as well as oxygen. This characteristic is similar to that of activated carbon. However, surface characteristics of the adsorbent could not be determined due to the failure of the equipment.

Adsorption potential of the leaves was also to be determined using high pressure tubular reactor as the adsorption column. Due to equipment failure, this objective could not be met. The suitable model for the adsorption of CO_2 on pentace triptera leaves can not be determined with certainty.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

5.1 CONCLUSION

Sips model showed a better fit to adsorption equilibrium data of CO_2 for the two adsorbents at all temperatures. This is because of the flexibility of the model which accounts for the heterogeneity of the surface of the adsorbent. Model parameters obtained form the data are in agreement with the observed behavior as found in literature. The heterogeneity of the sites of the adsorbent is showed by both the variation of Q with q and also by the value of c.

The potential of adsorption of CO_2 on pentace triptera leaves could not be determined due to equipment failure. It can not be concluded which adsorption isotherm model will be best to describe the adsorption of CO_2 on pentace triptera leaves

5.2 RECOMMENDATIONS

To increase the accuracy of data, more experimental data points should be studied. Data should be analyzed for at least 5 different temperatures.

To further add to the accuracy, it would be better to use the data that is obtained experimentally from the university laboratory. Uncertainties in experimental error add on to the modeling error during data correlation.

More models should be used to correlate data. Some models explore on several factors that are lacking or not addressed in the current study. Such data might be very useful in establishing a relationship between adsorbate and adsorbent during the process of adsorption.

To study the adsorption of CO_2 on pentace triptera leaves, volumetric apparatus can be constructed and set up as indicated in literature [2].

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APPENDICES

Appendix A : Equilibrium data for adsorption of CO_2 on molecular sieve 5A

Appendix B : Equilibrium data for adsorption of CO_2 on activated carbon

Appendix C : Data manipulation tool for Sips model

Appendix D : Nonlinear regression plots obtained for Sips model

Appendix E : Sample calculation for Langmuir parameters

Appendix F : Data for plotting of isosteric heats for adsorption on molecular sieve 5A

Appendix G : Data used for plotting isosteric heats for adsorption on activated carbon

Appendix H : Gantt chart

APPENDIX A

Table A-1: Equilibrium data for adsorption of CO_2 on molecular sieve 5A.

Pressure (KPa)	Amount adsorbed (mmol/g)		
	T=303K	T=373K	T=573K
0	0	0	0
40	1.606	1.244	0.083
80	2.548	1.815	0.169
120	3.068	2.121	0.239
160	3.332	2.412	0.291
200	3.448	2.642	0.33
240	3.467	2.737	0.361
280	3.474	2.808	0.41
320	3.48	2.865	0.438
360	3.484	2.91	0.493
400	3.485	2.948	0.537
440	3.492	2.979	0.598
480	3.495	3.006	0.639
520	3.497	3.028	0.688
560	3.498	3.048	0.731
600	3.506	3.066	0.774
640	3.515	3.081	0.82
680	3.523	3.095	0.837
720	3.528	3.107	0.861
760	3.532	3.119	0.901
800	3.538	3.129	0.938
840	3.545	3.138	0.967
880	3.544	3.146	0.992
920	3.545	3.154	1.012
960	3.546	3.161	1.031
1000	3.551	3.168	1.039

Table A-2: Data used to fit the Langmuir isotherm for molecular sieve 5A

Pressure KPa	**Pressure/ quantity adsorbed**		
	T = 303K	**T = 373K**	**T = 573K**
0	0	0	0
40	24.91	32.2	481.9
80	31.40	44.1	473.4
120	39.11	56.6	502.1
160	48.02	66.3	549.8
200	58.00	75.7	606.1
240	69.22	87.7	664.8
280	80.60	99.7	682.9
320	91.95	111.7	730.6
360	103.33	123.7	730.2
400	114.78	135.7	744.9
440	126.00	147.7	735.8
480	137.34	159.7	751.2
520	148.70	171.7	755.8
560	160.09	183.7	766.1
600	171.14	195.7	775.2
640	182.08	207.7	780.5
680	193.02	219.7	812.4
720	204.08	231.7	836.2
760	215.18	243.7	843.5
800	226.12	255.7	852.9
840	236.95	267.7	868.7
880	248.31	279.7	887.1
920	259.52	291.7	909.1
960	270.73	303.7	931.1
1000	281.61	315.7	962.5

APPENDIX B

Table B-1: Equilibrium data for adsorption of CO_2 on activated carbon

Pressure (Torr)	Quantity adsorbed	Pressure/Quantity adsorbed
0	0	0
100	0.7	142.86
200	1.12	178.57
300	1.5	200.00
400	1.72	232.56
550	2.2	250.00
652	2.31	282.25
750	2.7	277.78

Table B-2: Adsorption data of CO_2 on activated carbon at 373K

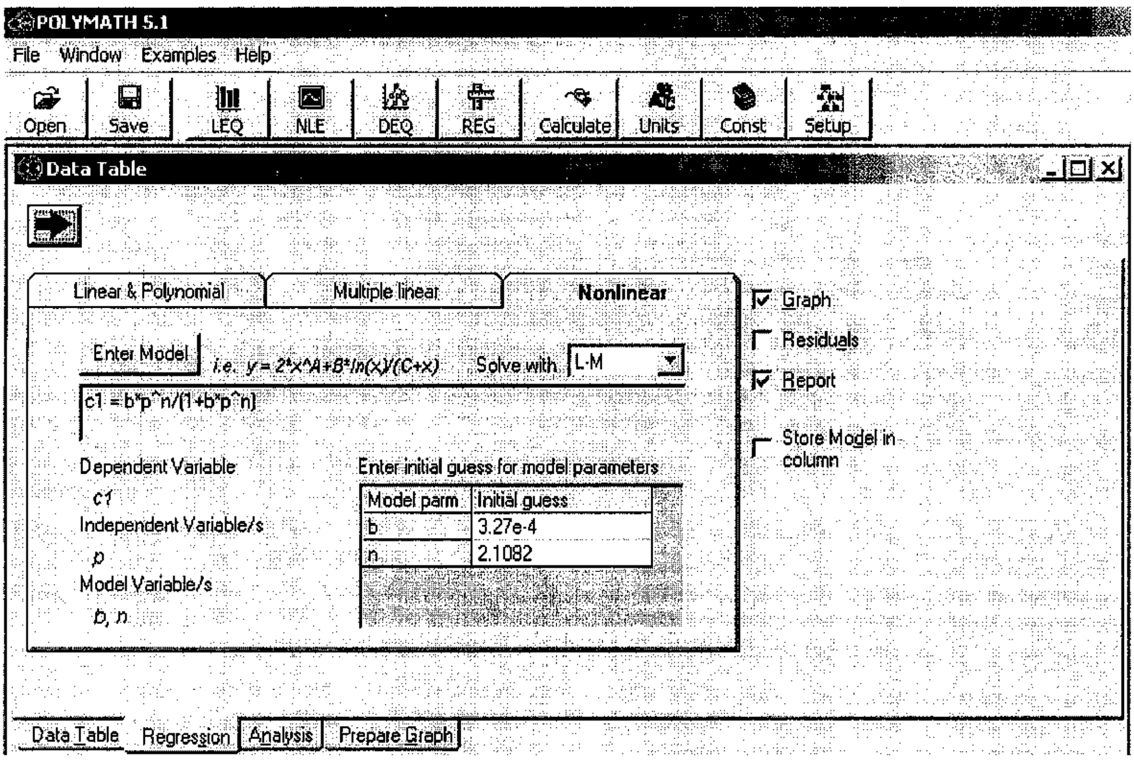
Pressure (Torr)	Quantity adsorbed	Pressure/Quantity adsorbed
0	0	0
125	0.3	416.7
200	0.5	400.0
300	0.6	500.0
475	0.625	760.0
640	0.78	820.5
725	0.875	828.6

Table B3: Adsorption data of CO_2 on activated carbon at 573K

Pressure (Torr)	**Quantity adsorbed**	**Pressure/Quantity adsorbed**
0	0	0
100	0.247	404.86
180	0.25	720.00
300	0.26	1153.85
450	0.28	1607.14
550	0.282	1950.35
700	0.313	2236.42

APPENDIX C

DATA MANIPULATION TOOL FOR MODELLING



*i.e. y = 2*X^A+B*ln(X)/(C+X)*

Solve with: L-M

```
c1 = b*p^n/(1+b*p^n)
```

Dependent Variable: *c1*

Independent Variable/s: *p*

Model Variable/s: *b, n*

Enter initial guess for model parameters

Model parm	Initial guess
b	3.27e-4
n	2.1082

☑ Graph
☐ Residuals
☑ Report
☐ Store Model in column

APPENDIX D

NON-LINEAR REGRESSION GRAPHS FROM SIPS MODEL.

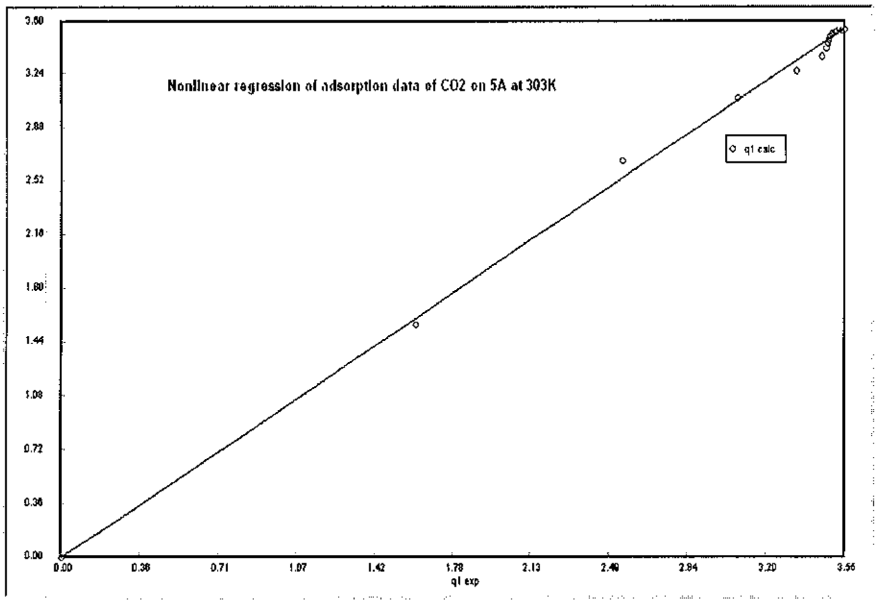


Figure D-1: Nonlinear regression graph for adsorption data of CO_2 on molecular sieve at 303K

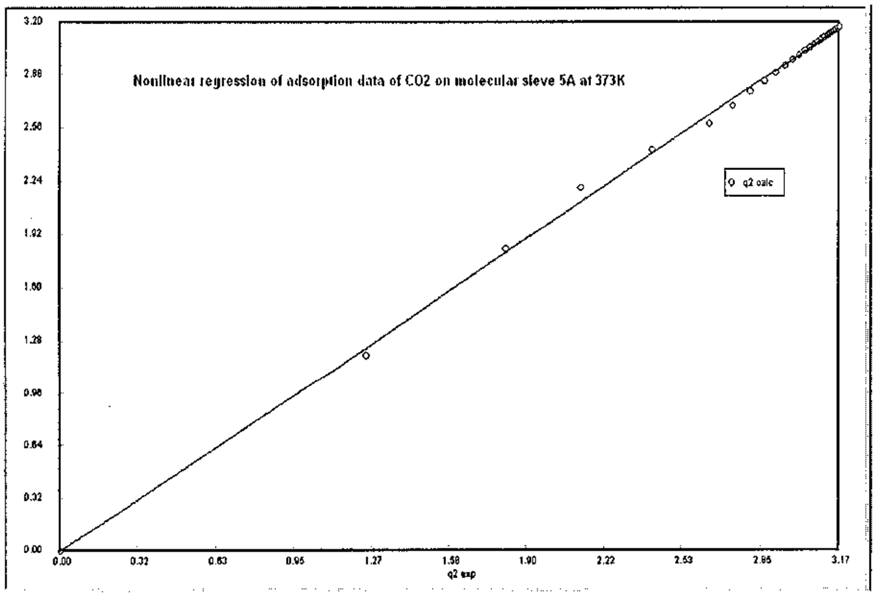


Figure D-2: Nonlinear regression graph for adsorption data of CO_2 on molecular sieve at 373K

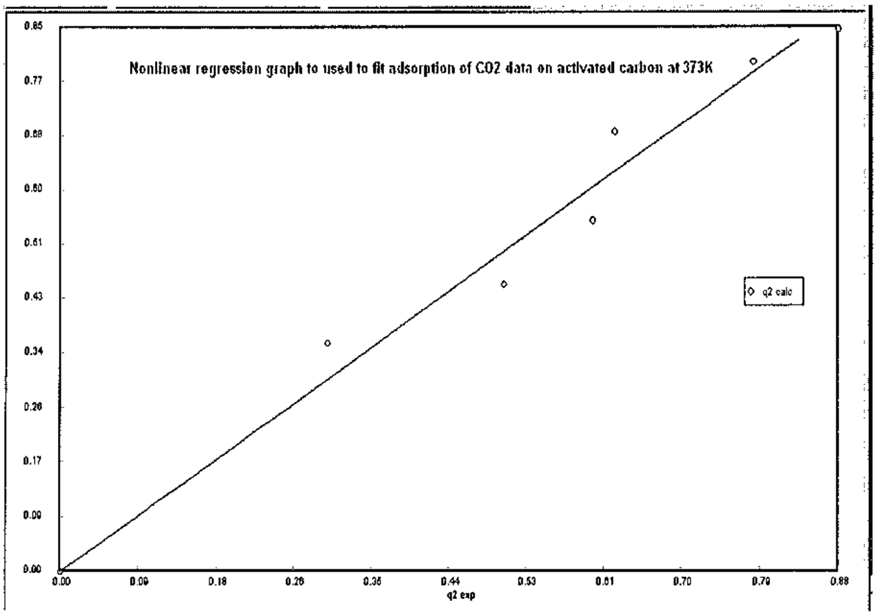


Figure D-5: Nonlinear regression graph for adsorption data of CO_2 on activated carbon at 373K

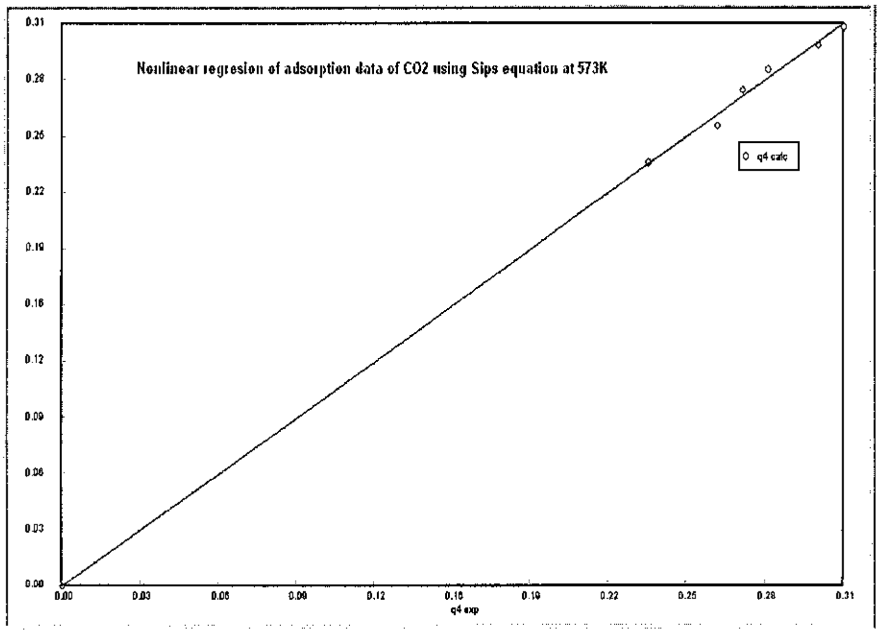


Figure D-6: Nonlinear regression graph for adsorption data of CO_2 on activated carbon at 573K

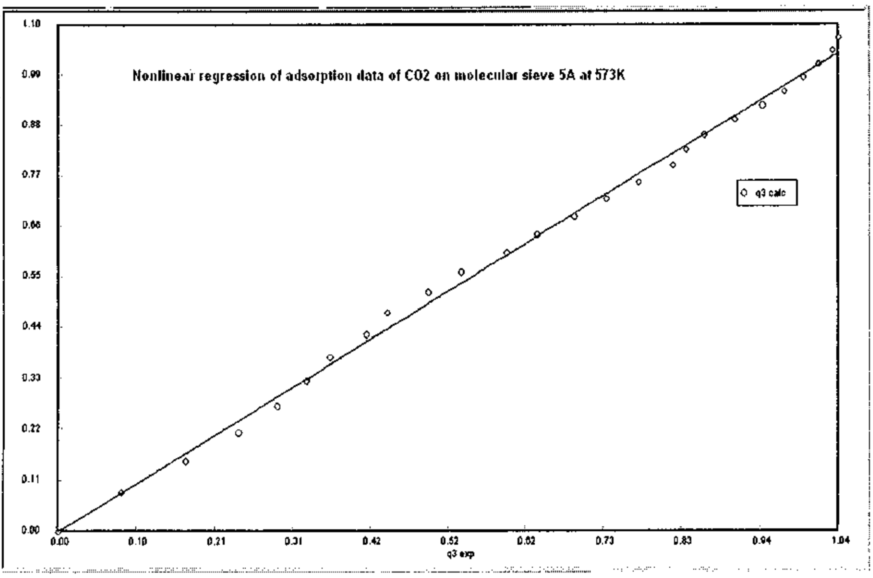


Figure D-3: Nonlinear regression graph for adsorption data of CO_2 on molecular sieve at 573K

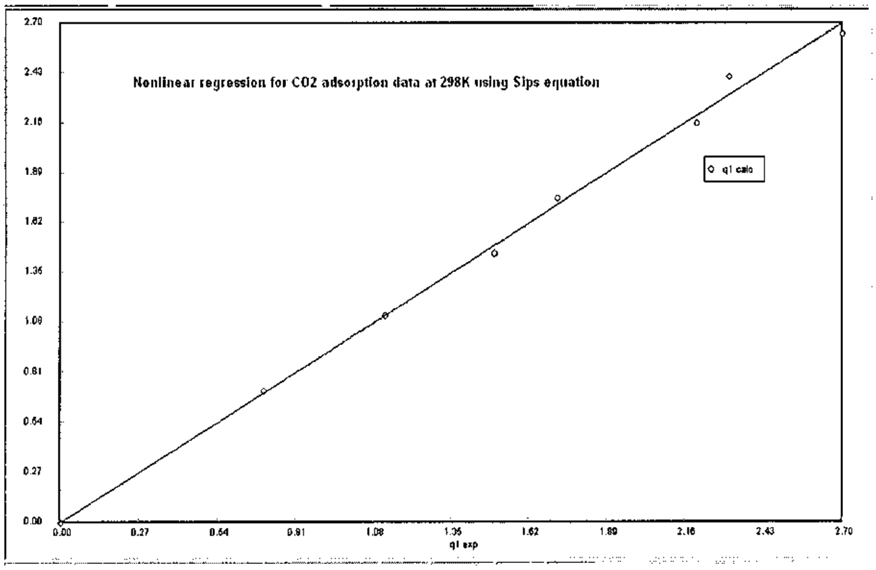


Figure D-4: Nonlinear regression graph for adsorption data of CO_2 on activated carbon at 298K

APPENDIX E

CALCULATION USED TO DETERMINE LANGMUIR PARAMETERS

For the equation:

y = 3.2442x + 96.55, which is in the form of:

$$\frac{p}{q} = \frac{1}{Kq_m} + \frac{p}{q_m}$$

The slope of the graph is $\frac{1}{q_m} = 3.2442$

$q_m = 1/3.2442 =$
$= 0.308$ mmol/g

Intercept = $\frac{1}{Kq_m} = 96.55$

$K = 1/(q_m * 96.55) = 0.034$

APPENDIX F

DATA FOR CALCULATION OF ISOSTERIC HEAT OF ADSORPTION FOR MOLECULAR SIEVE

Table F-1: Amount adsorbed at different pressures for Molecular Sieve 5A at 303K

Amount Adsorbed, q Mmol/g	**Pressure (KPa)**	**ln P KPa**
0	0	0
0.78	12.5	2.526
1.5	18.8	2.934
2	50	3.912
2.5	80	4.382
3	112.5	4.723
3.25	150	5.011

Table F-2: Amount adsorbed at different pressures for Molecular Sieve 5A at 373K

Amount adsorbed, q mmol/g	**Pressure, P KPa**	**ln P, KPa**
0	0	0
0.775	18.8	2.934
1.5	25	3.219
2	87.5	4.472
2.5	200	5.298
3	450	6.109
3.25	987	6.895

Table F-3: Amount adsorbed at different pressures for Molecular Sieve 5A at 573K

Amount adsorbed, q (mmol/g)	**Pressure, P (KPa)**	**ln P KPa**
0	0	0
0.775	600	6.397
1.5	920	6.824

APPENDIX G

DATA FOR CALCULATION OF ISOSTERIC HEAT OF ADSORPTION FOR ACTIVATED CARBON

Table G-1: Amount adsorbed at different pressures for activated carbon at 298K

Amount adsorbed, q Mmol/g	Pressure, P KPa	ln P KPa
0	0	0
0.233	13	2.565
0.25	13.3	2.588
0.27	14	2.639
0.28	16.6	2.809
0.3	23	3.135
0.31	26.7	3.285
0.5	53.3	3.976
0.66	80	4.382
0.86	120	4.787

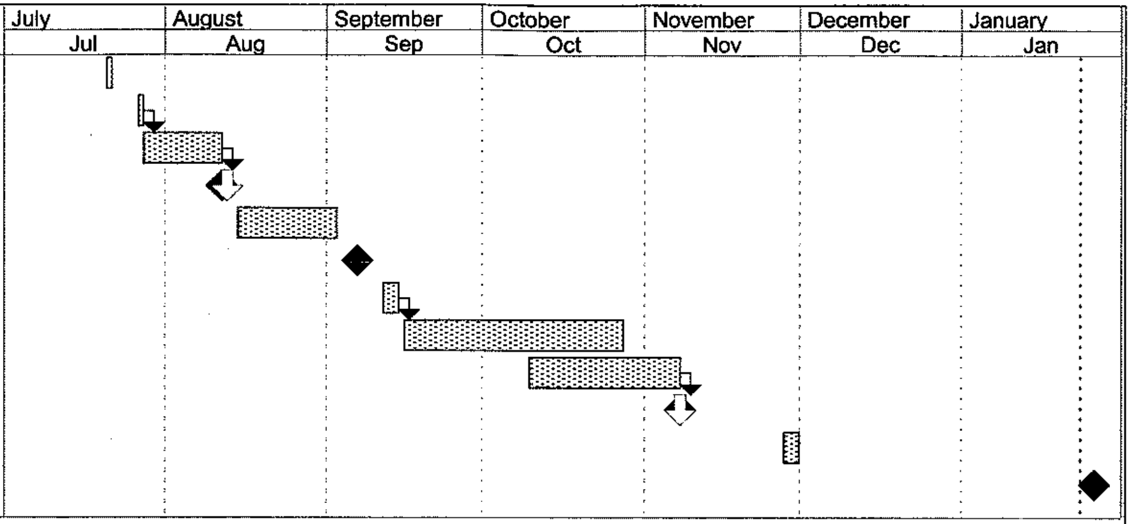
Table G-2: Amount adsorbed at different pressures for activated carbon at 373K

Amount adsorbed, q mmol/g	**Pressure , P KPa**	**ln P KPa**
0	0	0
0.233	73	4.290
0.25	83.3	4.422
0.27	95.8	4.562
0.28	100	4.605
0.3	113	4.727
0.31	120	4.787
0.5	273	5.609
0.66	550	6.310

Table G-3: Amount adsorbed at different pressures for activated carbon at 573K

Amount adsorbed, q mmol/g	**Pressure, P KPa**	**ln P KPa**
0	0	0
0.233	100	4.605
0.25	180	5.193
0.27	300	5.704
0.28	400	5.991
0.3	550	6.310
0.31	700	6.551

ID	Task Name	Duration	Start
1	Selection of Project	1 day	Thu 7/21/05
2	First meeting with supervisor	1 day	Wed 7/27/05
3	Preliminary Literature Review	11 days	Thu 7/28/05
4	Submission of Preliminary Report	0 days	Fri 8/12/05
5	Collection and Preparation of adsorbent	15 days	Mon 8/15/05
6	Submission of Progress Report	0 days	Wed 9/7/05
7	Collection of Data for modeling	3 days	Mon 9/12/05
8	Project work continue	30 days	Fri 9/16/05
9	Preparation of Dissertation Draft	21 days	Mon 10/10/05
10	Submission of Dissertation Final Draft	0 days	Mon 11/7/05
11	Oral Presentation	3 days	Mon 11/28/05
12	Submission of Hardbound copy of Project Dissertation	0 days	Fri 1/27/06



Project: FinalYrProject
Date: Tue 1/24/06

Task	▨	Rolled Up Task	▨	External Tasks	▨
Progress	▬	Rolled Up Milestone	◇	Project Summary	▬
Milestone	◆	Rolled Up Progress	▬	Group By Summary	▬
Summary	▬	Split	....	Deadline	⇩