CHAPTER 5

RESULTS AND DISCUSSIONS

The experimental results of this work are presented as follows:

5.1 Adsorption isotherms

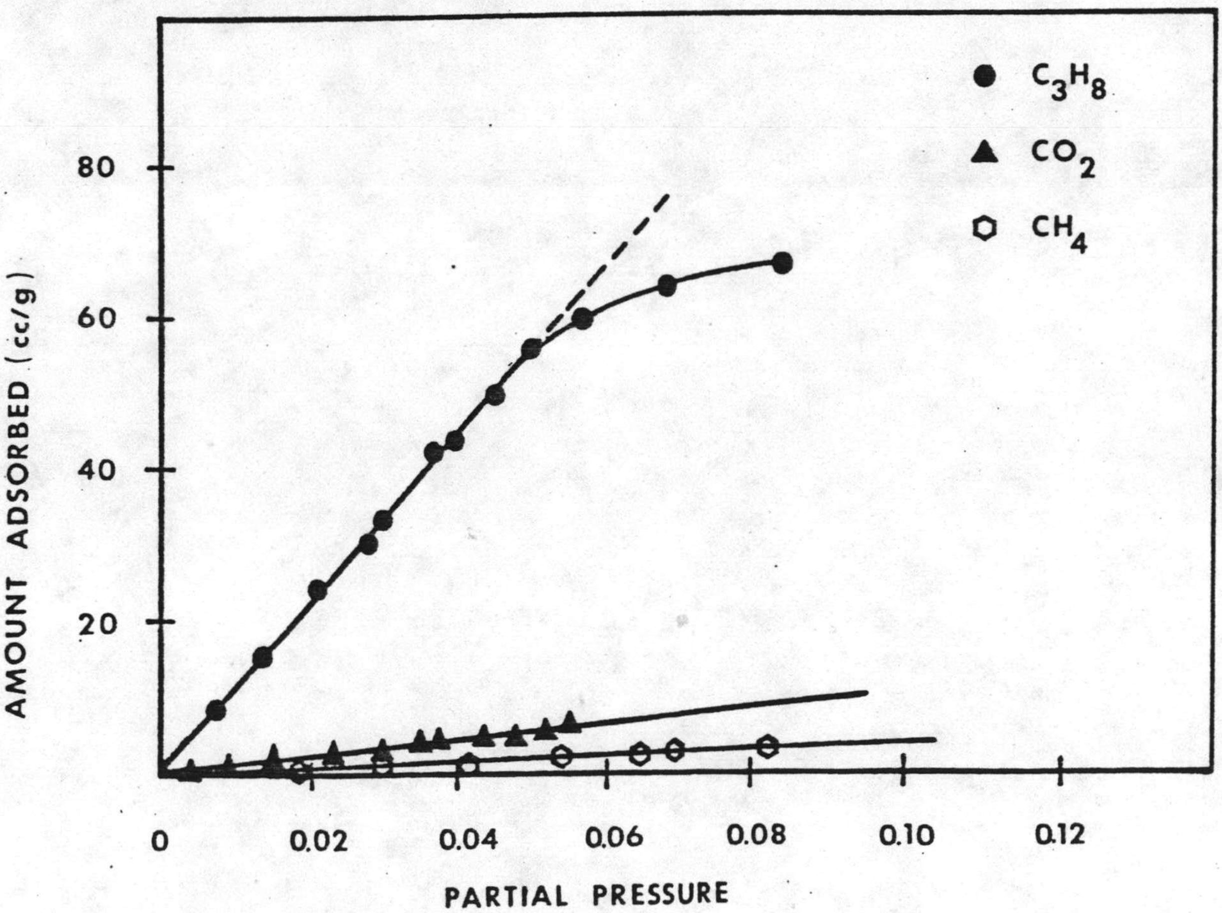

Figure 5.1 The adsorption isotherms of methane, carbondioxide, and propane on molecular sieve carbon - 5A at 45 °C.

5.1.1 Adsorption isotherms of single components.

The results of the experiments of the adsorption isotherms of carbondioxide , methane , and propane onto molecular sieve carbon -5A at 45 ° C and at the total pressure of 1 bar have been presented in figure 5.1.

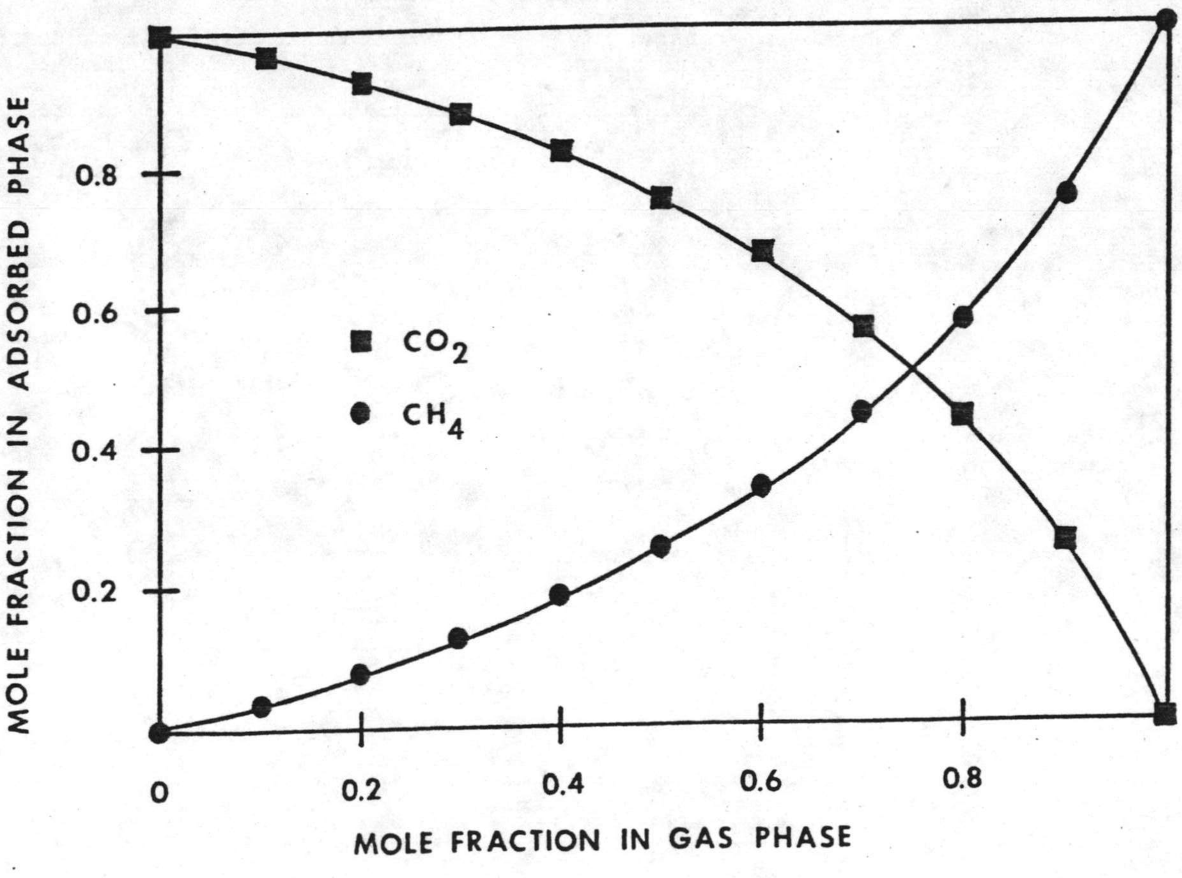

Figure 5.2 The adsorption isotherms of mixtures of carbondioxide and methane at 45 ° C and total pressure of Ø.5 bar.(Isotherms predicted using the ideal solution theory based on isotherms of pure components).

5.1.2 Adsorption isotherms of binary mixture.

The equilibrium adsorption isotherms of mixtures between carbondioxide and methane and between carbondioxide and propane on molecular sieve carbon -5A at 45 °C and at a total pressure of 0.5 bar are presented in figures 5.2 and 5.3 respectively. These curves are predicted by the ideal solution theory[ ]. The equilibrium curves of low concentration of hydrocarbons obtained by the chromatographic curves are shown in appendix A.

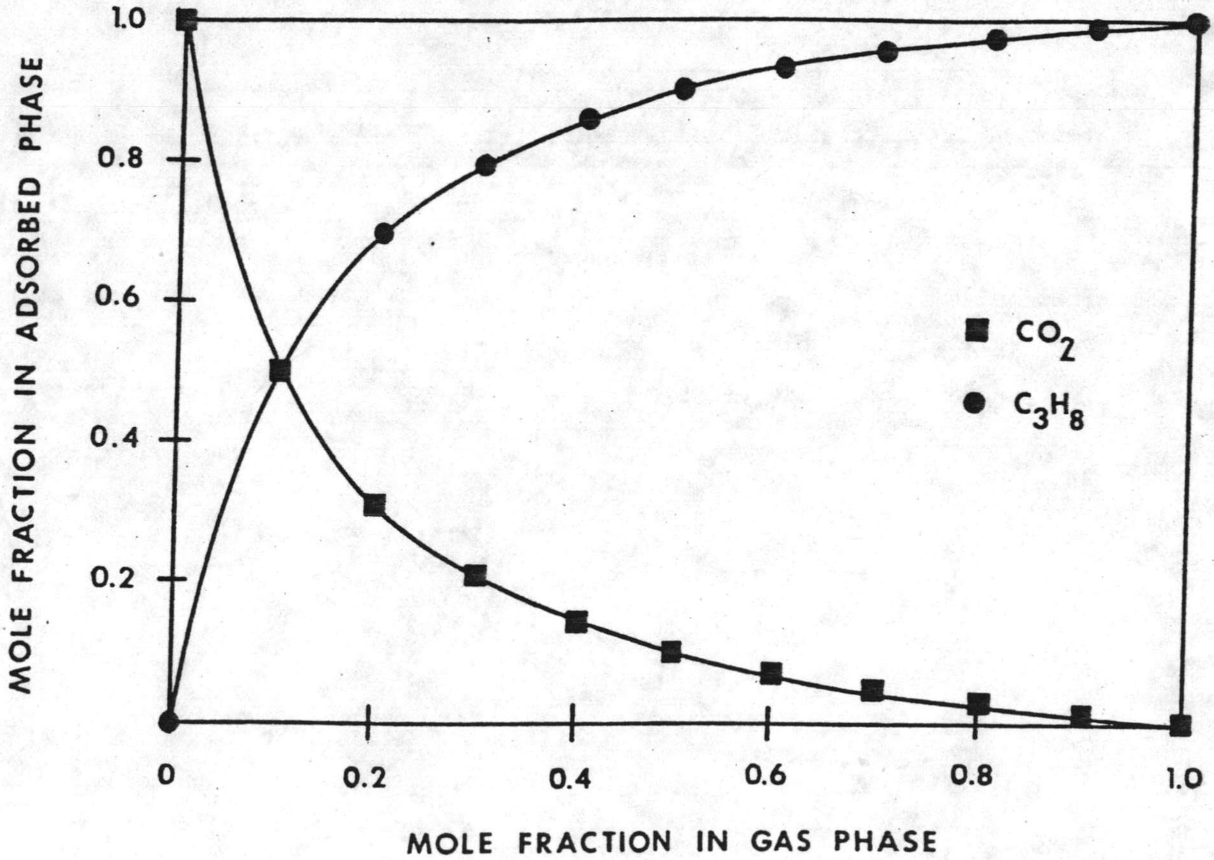

Figure 5.3 The adsorption isotherms of mixtures of carbondioxide and propane at 45 °C and 0.5 bar.(Isotherms predicted using the ideal solution theory based on isotherms of pure components)

5.2 The adsorption rate constants.

Measurements of equilibrium constants , binary molecular diffusivities , mass transfer coefficients , axial dispersion coefficients , adsorption rate constants ,and intraparticle diffusion coefficients based on the experiments are presented as follows :

5.2.1 Equilibrium constants.

The equilibrium constants obtained from equilibrium adsorption measurement (adsorption isotherms) and from evaluation of chromatographic peaks (moments method) are shown in table IV

TABLE IV

Adsorption coefficients on MSC -5A

TEMPERATURE 45 ° C and PRESSURE 1 BAR

Gas sample	K_A From equilibrium adsorption measurements	K_A (cc/g.MSC -5A) From evaluation of chromatographic peaks
METHANE	37.5	39.2753
CARBONDIOXIDE	113.0435	118.9546
PROPANE	1111.1111	1053.0756

5.2.2 The binary molecular diffusivities (D_{AB}).

The calculated binary molecular diffusivity of argon - methane , argon - carbondioxide , and argon - propane are presented in table V.(the calculations are shown in appendix G)

TABLE V

Binary molecular diffusivities at 45 ° C

BINARY MIXTURE	BINARY MOLECULAR DIFFUSIVITY (cm^2/min)
ARGON - METHANE	14.16
ARGON - CARBONDIOXIDE	9.468
ARGON - PROPANE	6.876

5.2.3 The mass transfer coefficients.

The calculated external mass transfer coefficients of methane , carbondioxide , and propane in the packed column of molecular sieve carbon - 5A are presented in table VI.(the calculations are shown in appendix G)

5.2.4 The axial dispersion coefficients.

The measured axial dispersion data of methane , carbondioxide , and propane in the packed bd of molecular sieve carbon - 5A at 45 ° C are presented in table VII.

TABLE VI

Measured mass transfer coefficients

TEMPERATURE 45 ° C and PRESSURE 1 BAR

	PARTICLE RADIUS (cm)	GAS METHANE	CARBONDIOXIDE	PROPANE
MASS TRANSFER	.0674	210.1070	140.4870	102.0151
COEFFICIENTS	.0940	150.6300	100.7180	73.1448
(cm/min)	.1204	117.6450	78.6607	57.1277

TABLE VII

Measured axial dispersion coefficients

	PARTICLE RADIUS (cm)	GAS METHANE	CARBONDIOXIDE	PROPANE
AXIAL DISPERSION	.0674	$1.6229*10^3$	$6.0036*10^2$	$2.0917*10^6$
COEFFICIENTS	.0940	$9.4512*10^2$	$3.8573*10^2$	$1.4172*10^6$
(cm^2/min)	.1204	$2.9491*10^2$	$1.3780*10^2$	$7.9152*10^5$

5.2.5 The adsorption rate constants.

The adsorption rate constants obtained from the moments analysis of a square pulse of methane , carbondioxide , and propane through the packed column of molecular sieve carbon - 5A are presented in table VIII.

TABLE VIII

Measured adsorption rate constants at 45 ° C

	PARTICLE RADIUS (cm)	GAS METHANE	CARBONDIOXIDE	PROPANE
ADSORPTION	.0674	624.3208	538.1124	734.9415
RATE CONSTANTS	.0940	569.8414	491.1558	670.8092
(cc/g.min)	.1204	541.6625	466.8678	637.6373
AVERAGE		578.6082	498.7120	681.1293

5.2.6 The intraparticle diffusion coefficients.

The measured intraparticle diffusion coefficients of methane , carbondioxide , and propane in the packed bed of molecular sieve carbon - 5A at 45 ° C are presented in table IX.

TABLE IX

Measured intraparticle diffusion coefficients

TEMPERATURE 45 °C and PRESSURE 1 BAR

	PARTICLE RADIUS		GAS	
	(cm)	METHANE	CARBONDIOXIDE	PROPANE
INTRAPARTICLE	.0674	.0299	.2159	.3982
DIFFUSION COEFF.	.0940	.0273	.1951	.3545
(cm^2/min)	.1204	.0259	.1845	.3327

5.3 Discussions

5.3.1 The adsorption isotherms.

The adsorption isotherms of single components as shown in figure 5.1 indicate that molecular sieve carbon – 5A adsorb preferentially propane , then carbondioxide and methane respectively. On the other hand the amount of pure gases adsorbed on molecular sieve carbon - 5A increase with molecular weights of each gas.

At very low partial pressures of methane , carbondioxide , and propane the adsorption isotherms are straight lines.

The equilibrium curve for adsorption of mixtures between carbondioxide and methane shown in figure 5.2 indicate that the amount of carbondioxide in the adsorbed phase increases rapidly at very low partial pressures but the amount of methane in the adsorbed phase increases very slowly. But the equilibrium curve for mixtures of carbondioxide and propane in figure 5.3 show that the amount of propane in the adsorbed phase increases rapidly while the amount of carbondioxide in adsorbed phase increases very slowly.

5.3.2 The equilibrium constants.

The equilibrium constants from the equilibrium adsorption measurements agree well with that evaluated from chromatographic peaks. The percentage difference between these two methods is only 4.52 , 4.97 , and 5.22 percent for methane , carbondioxide , and propane respectively. However these equilibrium adsorption constants can be used only in the low concentration region of the adsorbed gas. The equilibrium constants of ethane , propane , and n-butane adsorbed on silica gel at 50 $^\circ$ C studied by P. Schneider and J.M. Smith are shown in table X . The percentage difference between the two methods for the equilibrium constants is only 1 % for ethane and n-butane and 3 % for propane. The equilibrium constants obtained in this study have the same range than that obtained by P. Schneider and J.M. Smith [9].

5.3.3 The axial dispersion coefficients.

The axial dispersion coefficient cannot be depicted in this way , because its significance changes with the rate of flow of the carrier gas. Measured axial dispersions of gases passing through the packed column decrease when adsorbent particles become larger which is in agreement with known trends[21].

5.3.4 The adsorption rate constants.

The adsorption rate constants increase with molecular weight for hydrocarbon gases. However carbondioxide gas has the lowest adsorption rate constant compare with methane and propane.

TABLE X

Adsorption coefficients on silica gel at 50° C [9]

	Adsorption coefficient , K_A (cc/g SiO_2)	
Hydrcarbons	From equilibrium adsorption measurements	From evaluation of chromatographic peaks
ethane	14.5	14.6
propane	63	65.4
n-butane	308	311

If the hydrocarbon gas molecules are not larger than the pore diameters of the particles their adsorption rate constants will increase with molecular weight. But when the gas molecules are larger than the pore diameter of the particles they cannot pass through the pore and cannot be adsorbed on the adsorbent surface. This case indicates that smaller molecules will be preferentially adsorbed.

The adsorption rate constants of ethane , propane , and n-butane adsorbed on silica gel at 50 ° C as studied by P. Schneider and J.M. Smith are shown in table XI.

TABLE XI

The adsorption rate constants for ethane , propane , and n-butane from the data of P. Schneider and J.M. Smith [9].

Substance	k_{ads} (50° C) cc/g SiO_2
ethane	167
propane	255
n-butane	1500

The adsorption rate constants in table XI are in the same range as those obtained in this study.

5.3.5 The intraparticle diffusion coefficients.

The value of the intraparticle diffusion coefficients increase with molecular weight of the gases passing through the adsorption column. Compared to other parameters we can see that the intraparticle diffusion coefficient is very very low. Thus the intraparticle diffusion coefficient should be the rate determining step. Then we can use equation 3.10 to predict breakthrough curves and adsorption isotherms of methane , propane , and carbondioxide.

The intraparticle diffusion coefficients of ethane , propane , and n-butane adsorbed on silica gel at 50 °C studied by P.Schneider and J.M. Smith are in the same range as those obtained in this study. The values of the intraparticle diffusion coefficients obtained by P.Shneider and J.M. Smith[9] are shown in table XII.

TABLE XII

The intraparticle diffusion coefficients for ethane , propane , and n-butane (as measured by P. Schneider and J.M. Smith [9])

Hydrocarbon	$D_c \times 10^3$ (sq.cm./sec)
ethane	1.41
propane	1.54
n-butane	2.93

The parameters obtained were used to predict C(Z,t) using equations 3.10 - 3.21. The results of the calculation of C(Z,t) compared to the results from the experimental data for methane , carbondioxide , and propane are shown in figure

5.4 , 5.5 , and 5.6 respectively. The results show that the agreement between the experimental and predicted breakthrough curves is excellent. This is perhaps surprising since the prediction method neglects axial dispersion although in the previous section it had been shown that axial dispersion did play some influence on the chromatographic wave.

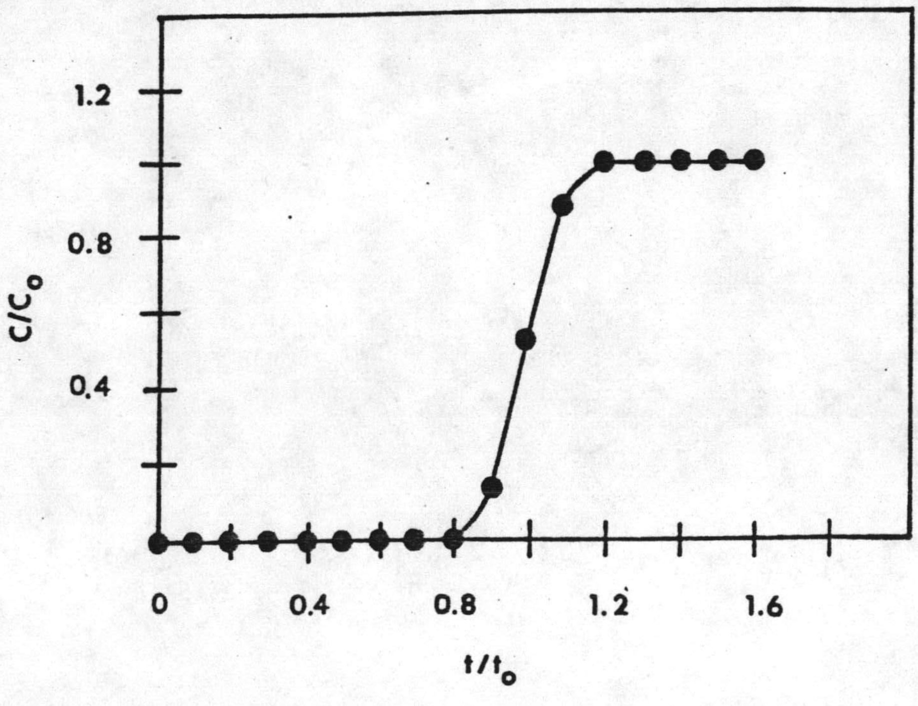

Figure 5.4 Breakthrough curves of methane at a flowrate of Ø.173 cc/sec and a concentration of .Ø2 cc/cc-argon.(Points denote experimental data ; solid lines are predicted curves)

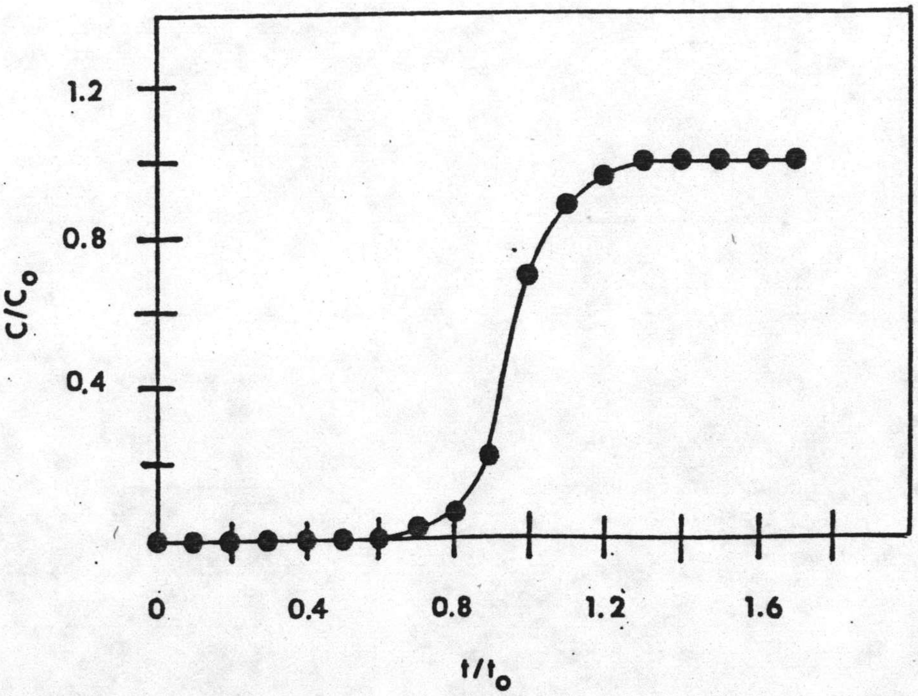

Figure 5.5 Breakthrough curves of propane at a flowrate of 6.7385 cc/sec and a concentration of .02 cc/cc-argon.(Points denote experimental data ; solid lines are predicted curves)

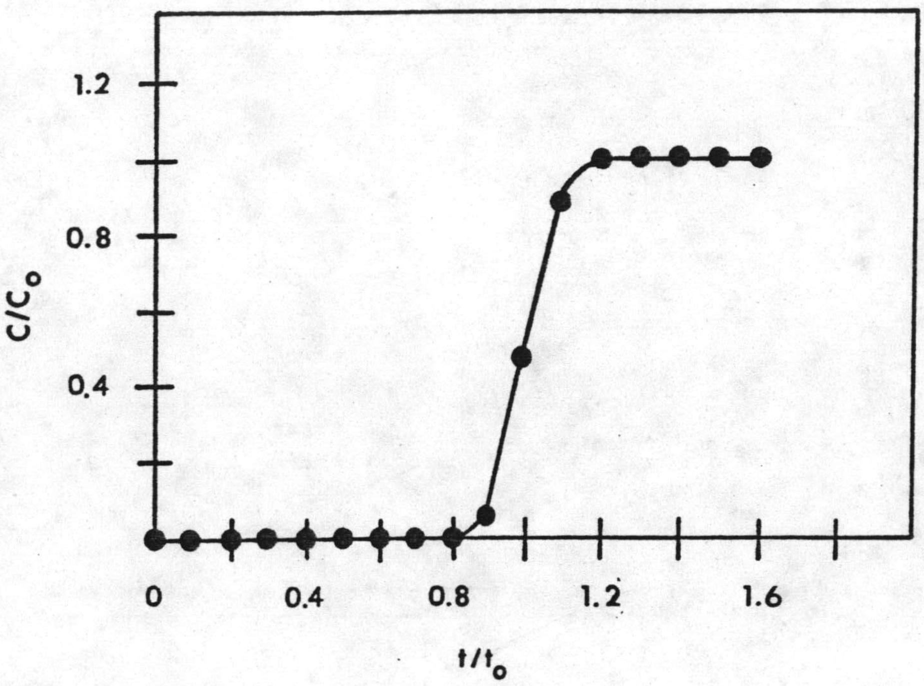

Figure 5.6 Breakthrough curves of carbondioxide at a flowrate of Ø.3226 cc/sec and a concentration of .Ø35 cc/cc-argon.(Points denote experimental data ; solid lines are predicted curves)