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NOTATION

$\emptyset_A$ cross sectional area of adsorption column

C concentration of the adsorbable gas in the interparticle space , mole/ml.

C_{ads} concentration of the adsorbable gas in the adsorbed phase , mole/ml.

C_1 concentration of the adsorbable gas in the pore space , mole/ml.

C_o concentration of the adsorbable gas in the input concentration function , mole/ml.

D_c effective intraparticle diffusion coefficient defined as the ratio of the diffusional flux through a unit area of the geometrical surface of the particle to the negative of the intraparticle concentration gradient , sq. cm./sec.

E_A effective axial dispersion coefficient , defined as the ratio of the axial diffusional flux through the unit area of the the total cross section of the column to the negative of the interparticle concentration gradient , sq.cm./sec.

k_{ads} adsorption rate constant , ml/g.sec.

k_f mass transfer coefficient , cm/sec.

K adsorption equilibrium constant , ml/g

N diffusional flux

r length coordinate in the spherical particle of adsorbent

, cm.

R   radius of the spherical particle of adsorbent , cm.

s   Laplace - Carson transform variable

t   time , sec.

t_o time of duration of the injection of the adsorbable gas , sec.

T   absolute temperature

v   linear velocity of the carrier gas in the interparticle space , cm./min.

y   integration variable

Z   length coordinate of the bed of adsorbent , cm.

α interparticle void fraction in the adsorbent bed

β intraparticle void fraction of the adsorbent

ρ_p apparent particle density , g./ml.

APPENDIX

APPENDIX A

DATA OF THE CHROMATOGRAPHIC CURVES

TABLE A1

The output of the ten minutes square pulses of methane passing through the packed column (average particle radius 0.1204 cm).

	concentration(%)			
time (min)	$Z/v = 0.1371$	0.2917	0.3938	0.6070
1	0	0	0	0
2	0.1150	0	0	0
3	0.8341	0	0	0
4	0.9396	0	0	0
5	0.9204	0.3739	0	0
6	0.9012	0.8916	0.1246	0
7	0.9204	0.9204	0.6519	0
8	0.9012	0.9024	0.9204	0
9	0.9204	0.9587	0.9396	0.0096
10	0.9012	0.9396	0.9587	0.1630
11	0.9012	0.9396	0.9204	0.5657
12	0.8820	0.9204	0.9204	0.9012
13	0.4794	0.9204	0.9012	0.9396
14	0.1747	0.9012	0.8820	0.9587
15	0.1438	0.7191	0.9012	0.9396
16	0.0575	0.3739	0.9012	0.9396
17	0.0288	0.1630	0.6903	0.8820
18	0.0096	0.1438	0.3835	0.9204
19	0.0038	0.0863	0.2301	0.9012
20	0.0000	0.0383	0.1150	0.7862
21		0.0288	0.0479	0.6136
22		0.0288	0.0383	0.4218
23		0.0192	0.0383	0.2780
24		0.0192	0.0288	0.1630
25		0.0096	0.0288	0.0767
26		0.0096	0.0192	0.0479
27		0.0038	0.0192	0.0383
28		0.0038	0.0192	0.0383

29		0.0000	0.0096	0.0288
30			0.0096	0.0288
31			0.0096	0.0288
32			0.0038	0.0192
33			0.0038	0.0192
34			0.0038	0.0192
35			0.0000	0.0096
36				0.0096
37				0.0096
38				0.0038
39				0.0038
40				0.0038
41				0.0038
42				0.0000

TABLE A2

The output of the ten minutes square pulses of methane passing through the packed column (average particle radius 0.0940 cm).

	concentration(%)			
time (min)	Z/v = 0.1485	0.3167	0.4002	0.5440
1	0	0	0	0
2	0.0288	0	0	0
3	0.7478	0	0	0
4	0.9587	0	0	0
5	0.9587	0.1246	0	0
6	0.9204	0.6424	0.0671	0
7	0.9204	0.8437	0.4506	0
8	0.9204	0.8820	0.8149	0.0383
9	0.8820	0.8820	0.9204	0.2493
10	0.9396	0.9396	0.9396	0.6424
11	0.9012	0.9204	0.9204	0.8053
12	0.9012	0.9012	0.9396	0.8820
13	0.4794	0.9012	0.9012	0.9012
14	0.1438	0.9396	0.8820	0.9396
15	0.0575	0.8053	0.8629	0.9204
16	0.0288	0.5177	0.8149	0.8820
17	0.0192	0.2589	0.6232	0.9012
18	0.0096	0.1246	0.4027	0.9012

19	0.0000	0.0671	0.2109	0.7095
20		0.0479	0.1150	0.5561
21		0.0383	0.0671	0.3739
22		0.0288	0.0479	0.2205
23		0.0288	0.0383	0.1246
24		0.0192	0.0383	0.0671
25		0.0192	0.0288	0.0479
26		0.0096	0.0288	0.0479
27		0.0096	0.0192	0.0479
28		0.0096	0.0192	0.0383
29		0.0000	0.0192	0.0383
30			0.0096	0.0383
31			0.0096	0.0288
32			0.0096	0.0288
33			0.0038	0.0288
34			0.0038	0.0192
35			0.0038	0.0192
36			0.0000	0.0192
37				0.0096
38				0.0096
39				0.0096
40				0.0038
41				0.0038
42				0.0038
43				0.0000

TABLE A3

The output of the ten minutes square pulses of methane passing through the packed column (average particle radius 0.0674 cm).

		concentration(%)		
time (min)	Z/v = 0.1536	0.2602	0.4192	0.5797
1	0	0	0	0
2	0.0383	0	0	0
3	0.5561	0	0	0
4	0.8053	0.0383	0	0
5	0.9012	0.4985	0	0
6	0.9204	0.7670	0	0
7	0.9012	0.8053	0.0959	0

8	0.9204	0.9204	0.5177	0
9	0.8820	0.9012	0.8149	0.0959
10	0.9396	0.9396	0.9204	0.1438
11	0.9204	0.8820	0.9204	0.4985
12	0.8820	0.8820	0.9102	0.7862
13	0.4602	0.8820	0.9204	0.8245
14	0.1438	0.8053	0.8820	0.8820
15	0.0479	0.6136	0.9204	0.9587
16	0.0383	0.2876	0.9012	0.8916
17	0.0307	0.1342	0.8245	0.8820
18	0.0153	0.0767	0.6136	0.9012
19	0.0000	0.0383	0.3835	0.8820
20		0.0288	0.2109	0.7780
21		0.0192	0.0959	0.6232
22		0.0096	0.0767	0.4218
23		0.0038	0.0671	0.3010
24		0.0000	0.0479	0.1726
25			0.0383	0.0863
26			0.0288	0.0671
27			0.0192	0.0479
28			0.0038	0.0479
29			0.0038	0.0383
30			0.0000	0.0383
31				0.0288
32				0.0288
33				0.0192
34				0.0192
35				0.0096
36				0.0096
37				0.0038
38				0.0038
39				0.0000

TABLE A4

The output of the five minutes square pulses of carbondioxide passing through the packed column (average particle radius 0.1204 cm).

		concentration(%)		
time (min)	Z/v = 0.0945	0.1706	0.2563	0.4235

1	0	0	0	0
2	0	0	0	0
3	0.0383	0	0	0
4	0.3145	0	0	0
5	0.7325	0	0	0
6	0.9396	0	0	0
7	1.0584	0.0690	0	0
8	1.0584	0.3451	0	0
9	0.7823	0.7977	0	0
10	0.5752	0.8820	0	0
11	0.3835	0.8437	0.0307	0
12	0.2301	0.7670	0.2301	0
13	0.1419	0.6750	0.7286	0
14	0.0690	0.6443	0.8053	0
15	0.0537	0.4525	0.8360	0
16	0.0383	0.3145	0.8207	0
17	0.0230	0.2454	0.8053	0
18	0.0230	0.1534	0.7286	0
19	0.0077	0.0997	0.5522	0.0690
20	0.0038	0.0690	0.4679	0.1534
21	0.0000	0.0383	0.3758	0.3451
22		0.0230	0.2684	0.5752
23		0.0077	0.2109	0.7018
24		0.0038	0.1419	0.7210
25		0.0000	0.0997	0.7018
26			0.0767	0.6366
27			0.0690	0.5752
28			0.0614	0.5292
29			0.0460	0.4525
30			0.0307	0.3758
31			0.0153	0.3528
32			0.0077	0.2838
33			0.0038	0.2301
34			0.0000	0.1841
35				0.1381
36				0.1151
37				0.0959
38				0.0690
39				0.0652
40				0.0575

41	0.0499
42	0.0422
43	0.0345
44	0.0283
45	0.0192
46	0.0115
47	0.0038
48	0.0000

TABLE A5

The output of the ten minutes square pulses of carbondioxide passing through the packed column (average particle radius 0.0940 cm).

	concentration(%)			
time (min)	Z/v = 0.0725	0.1296	0.1989	0.2749
1	0	0	0	0
2	0	0	0	0
3	0.1687	0	0	0
4	0.7210	0	0	0
5	1.0278	0.1112	0	0
6	1.0584	0.4602	0	0
7	1.0354	0.7670	0	0
8	0.8820	0.9587	0.0307	0
9	0.6059	0.9894	0.1074	0
10	0.3451	0.9472	0.3451	0
11	0.1534	0.7363	0.6289	0
12	0.1074	0.6673	0.8514	0.0614
13	0.0460	0.4794	0.8667	0.1419
14	0.0307	0.3375	0.8590	0.2454
15	0.0153	0.2224	0.6826	0.3835
16	0.0077	0.1419	0.6213	0.5367
17	0.0000	0.1074	0.4909	0.7133
18		0.0614	0.3988	0.7593
19		0.0383	0.2953	0.7286
20		0.0153	0.2224	0.6136
21		0.0077	0.1534	0.4832
22		0.0000	0.1074	0.3988
23			0.0729	0.3451
24			0.0614	0.3221

25	0.0537	0.2454
26	0.0383	0.1994
27	0.0307	0.1381
28	0.0153	0.1074
29	0.0077	0.0920
30	0.0038	0.0767
31	0.0000	0.0620
32		0.0537
33		0.0383
34		0.0307
35		0.0153
36		0.0077
37		0.0038
38		0.0000

TABLE A6

The output of the five minutes square pulses of carbondioxide passing through the packed column (average particle radius 0.0674 cm).

	concentration(%)			
time (min)	Z/v = 0.0472	0.0915	0.1592	0.2300
1	0	0	0	0
2	0.0806	0	0	0
3	0.6673	0	0	0
4	1.0354	0.0307	0	0
5	1.0584	0.3451	0	0
6	1.0354	0.7670	0	0
7	0.9511	1.0009	0.0153	0
8	0.5944	1.0508	0.0997	0
9	0.3145	0.9971	0.3451	0
10	0.1457	0.7670	0.6289	0
11	0.0690	0.5446	0.7900	0.0575
12	0.0307	0.3797	0.8820	0.2071
13	0.0153	0.2186	0.7977	0.4717
14	0.0077	0.1381	0.6673	0.7440
15	0.0000	0.0767	0.5292	0.7977
16		0.0460	0.4103	0.8283
17		0.0307	0.3145	0.7977
18		0.0077	0.2378	0.7056

19	0.0000	0.1687	0.5944
20		0.1112	0.4909
21		0.0844	0.3758
22		0.0680	0.3221
23		0.0383	0.2454
24		0.0307	0.1764
25		0.0192	0.1381
26		0.0077	0.1035
27		0.0038	0.0652
28		0.0000	0.0537
29			0.0460
30			0.0383
31			0.0307
32			0.0230
33			0.0153
34			0.0077
35			0.0038
36			0.0000

TABLE A7

The output of the ten minutes square pulses of propane passing through the packed column (average particle radius 0.1204 cm).

$\div 1.3333$ time (min)	concentration $\times 10^3$ (mole/cc)			
	Z/v = 0.0125	0.0166	0.0221	0.0288
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0.3129	0	0	0
5	1.5906	0.5215	0	0
6	2.1643	1.4603	0	0
7	2.2947	2.2947	0.7301	0
8	1.9818	2.2947	1.5906	0.2151
9	1.7992	2.1122	2.2425	1.1473
10	1.1473	2.0861	1.9818	1.7210
11	0.7041	1.3820	1.5646	1.6687
12	0.5215	1.0691	1.3820	1.3820
13	0.4172	0.9127	0.9127	1.0691
14	0.3716	0.6258	0.7041	0.8084

15	0.3259	0.5215	0.6258	0.7138
16	0.2803	0.4172	0.5215	0.6193
17	0.2347	0.3564	0.4172	0.5247
18	0.2230	0.2955	0.3911	0.4303
19	0.1122	0.2347	0.3651	0.4064
20	0.1995	0.2253	0.3390	0.3825
21	0.1878	0.2159	0.3129	0.3585
22	0.1760	0.2065	0.2868	0.3347
23	0.1643	0.1971	0.2607	0.3108
24	0.1526	0.1877	0.2347	0.2869
25	0.1408	0.1783	0.2253	0.2630
26	0.1291	0.1690	0.2159	0.2391
27	0.1174	0.1596	0.2065	0.2151
28	0.1057	0.1502	0.1971	0.2069
29	0.0939	0.1408	0.1877	0.1986
30	0.0822	0.1314	0.1783	0.1903
31	0.0705	0.1220	0.1690	0.1821
32	0.0587	0.1126	0.1596	0.1738
33	0.0470	0.1032	0.1502	0.1655
34	0.0353	0.0938	0.1408	0.1572
35	0.0235	0.0844	0.1314	0.1490
36	0.0118	0.0751	0.1220	0.1407
37	0.0000	0.0657	0.1126	0.1324
38		0.0563	0.1032	0.1242
39		0.0469	0.0938	0.1159
40		0.0375	0.0844	0.1076
41		0.0281	0.0751	0.0994
42		0.0187	0.0657	0.0911
43		0.0093	0.0563	0.0828
44		0.0000	0.0469	0.0745
45			0.0375	0.0663
46			0.0281	0.0580
47			0.0187	0.0497
48			0.0093	0.0415
49			0.0000	0.0332
50				0.0249
51				0.0166
52				0.0038
53				0.0000

TABLE A8

The output of the ten minutes square pulses of propane passing through the packed column (average particle radius 0.0940 cm).

$\div$ 1.3333	concentration x10^3 (mole/cc)			
time (min)	Z/v = 0.0095	0.0121	0.0146	0.0183
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	1.4603	0.2151	0	0
5	1.9818	1.4603	0.7041	0
6	2.2947	2.1122	2.0600	0.5215
7	2.2947	2.2947	2.2947	1.8644
8	2.2947	2.2947	2.2947	2.2947
9	2.2947	2.0600	2.1643	2.1643
10	2.1122	1.7992	1.8644	2.1122
11	2.0861	0.9909	1.1473	1.6689
12	1.6167	0.6258	0.6258	1.1213
13	1.3820	0.5215	0.5215	0.6258
14	0.7041	0.4172	0.4172	0.5737
15	0.5215	0.3564	0.3564	0.5215
16	0.4172	0.2955	0.2955	0.4694
17	0.3807	0.2347	0.2347	0.4172
18	0.3442	0.2295	0.2249	0.3868
19	0.3077	0.2112	0.2151	0.3564
20	0.2712	0.1995	0.2053	0.3260
21	0.2347	0.1878	0.1956	0.2955
22	0.2179	0.1760	0.1858	0.2651
23	0.2012	0.1643	0.1760	0.2347
24	0.1844	0.1526	0.1662	0.2249
25	0.1676	0.1408	0.1564	0.2151
26	0.1509	0.1291	0.1467	0.2053
27	0.1341	0.1174	0.1369	0.1956
28	0.1174	0.1057	0.1271	0.1858
29	0.1006	0.0939	0.1173	0.1760
30	0.0838	0.0822	0.1075	0.1662
31	0.0671	0.0705	0.0978	0.1564
32	0.0503	0.0587	0.0880	0.1467
33	0.0336	0.0470	0.0782	0.1369

time	col1	col2	col3	col4
34	0.0168	0.0353	0.0684	0.1271
35	0.0000	0.0235	0.0586	0.1173
36		0.0118	0.0489	0.1075
37		0.0000	0.0391	0.0978
38			0.0293	0.0880
39			0.0195	0.0782
40			0.0974	0.0684
41			0.0000	0.0586
42				0.0489
43				0.0391
44				0.0293
45				0.0195
46				0.0097
47				0.0000

TABLE A9

The output of the ten minutes square pulses of propane passing through the packed column (average particle radius 0.0674 cm).

$\div$ 1.3333	concentration x10^3 (mole/cc)			
time (min)	Z/v = 0.0090	0.0111	0.0142	0.0175
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0.9909	0	0	0
5	2.1643	1.5124	0	0
6	2.2947	2.2947	1.6167	0
7	2.2947	2.2947	1.9818	1.5124
8	2.2947	2.1122	2.2947	2.2947
9	2.1643	1.9296	2.2947	2.2947
10	1.9818	1.3820	2.1122	2.1122
11	1.1213	0.9127	1.7992	1.6167
12	0.8083	0.6519	1.1473	1.3820
13	0.6258	0.6258	0.7041	1.0691
14	0.4172	0.5215	0.6258	0.9127
15	0.3564	0.4172	0.4172	0.7041
16	0.2955	0.3564	0.3716	0.6258
17	0.2347	0.2955	0.3259	0.5215
18	0.2223	0.2347	0.2803	0.4172

19	0.2100	0.2235	0.2347	0.3807
20	0.1976	0.2123	0.2230	0.3442
21	0.1853	0.2011	0.2112	0.3077
22	0.1729	0.1900	0.1995	0.2712
23	0.1606	0.1788	0.1878	0.2347
24	0.1482	0.1676	0.1760	0.2249
25	0.1359	0.1564	0.1643	0.2151
26	0.1235	0.1452	0.1526	0.2053
27	0.1112	0.1341	0.1408	0.1956
28	0.0988	0.1229	0.1291	0.1858
29	0.0865	0.1117	0.1174	0.1760
30	0.0741	0.1005	0.1057	0.1662
31	0.0618	0.0893	0.0939	0.1564
32	0.0494	0.0782	0.0822	0.1467
33	0.0371	0.0670	0.0705	0.1369
34	0.0247	0.0558	0.0587	0.1271
35	0.0124	0.0446	0.0470	0.1173
36	0.0000	0.0334	0.0353	0.1075
37		0.0223	0.0235	0.0978
38		0.0111	0.0118	0.0880
39		0.0000	0.0000	0.0782
40				0.0684
41				0.0586
42				0.0489
43				0.0391
44				0.0293
45				0.0195
46				0.0097
47				0.0000

APPENDIX B

THE DETERMINATION OF ADSORPTION RATE CONSTANTS

The outputs of square pulses passing through the packed column of molecular sieve carbon - 5A at 45 $^\circ$ C at a total pressure of 1 bar are presented in figure B1. The input square pulses have a carbondioxide concentration of about 1.0584 mole/cc and the square pulse time is 5 minutes long.
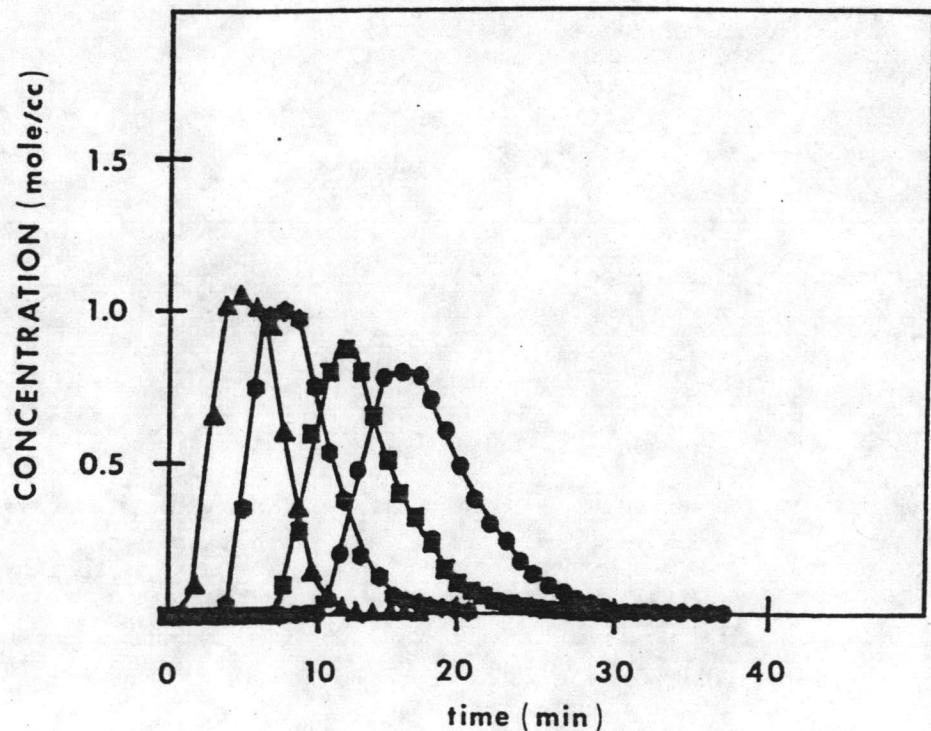
Figure B1 The output of a square pulse of carbondioxide at different flow rates of carrier gas.

From the output of the square pulse we can find the first moment and second central moment using the following program written in BASICA.

```
10  DIM Y(100)
20  CLS
30  INPUT "NO. OF DATA = ";M
40  E = 1
50  H = 1+(1/6)
60  FOR I = 1 TO M
70  PRINT "INPUT DATA NO ";I:INPUT Y(I)
80  NEXT I
90  GOSUB 420
100  PRINT "----------------------------------"
110  PRINT "T(MIN)              C(MOL/CC)"
120  PRINT "----------------------------------"
130  FOR I = 0 TO M
140  T = I
150  PRINT "    "T;TAB(26);Y(I)
160  NEXT I
170  PRINT "----------------------------------"
180  PRINT "TOTAL AREA = ";A;"   MOL.SEC/CC  "
190  IF E = 2 THEN PRINT "MUE1  =";A/EE
200  PRINT "----------------------------------"
210  INPUT "DO YOU WANT TO FIND THE OTHER MOMENT ";Z$
220  IF Z$ ="N"GOTO 290
230  E = 2  .
240  EE = A
250  FOR I = 0 TO M
260  Y(I) = I*Y(I)
270  NEXT I
280  GOTO 90
290  INPUT "DO YOU WANT TO CALCULATE CENTRAL MOMENT AGAIN ";Z$
300  IF Z$ = "Y" THEN GOTO 320
310  END
320  FOR I = 0 TO M
330  IF I = 0 GOTO 350
340  Y(I) = Y(I)/I
350  Y(I) = (I-A/EE)^2*Y(I)
360  NEXT I
370  GOSUB 420
380  PRINT "CENTRAL MOMENT =";A/EE
390  INPUT "DO YOU WANT TO CALCULATE CENTRAL MOMENT AGAIN ";Z$
400  IF Z$ = "Y" THEN GOTO 20
410  GOTO 310
420  A = 0 : IS =1
430  IF (2*INT(M/2) = M) THEN GOTO 470
440  A = (3*H/8)*(Y(0) + 3*Y(1) + 3*Y(2) + Y(3))
450  IS = 5
460  IF M = 3 THEN GOTO 520
470  A = A + (H/3) * (Y(IS-1) + 4*Y(M-1) + Y(M))
480  IF IS > M-2 THEN GOTO 520
490  FOR I = IS TO M-2 STEP 2
500  A = A + (H/3) * (4*Y(I) + 2*Y(I+1))
510  NEXT I
520  RETURN
```

The first moment from the square pulse will give a reduced moment and the Z/V curve as shown in figure B2 which gives the equilibrium constant based on the slopes of these curves.
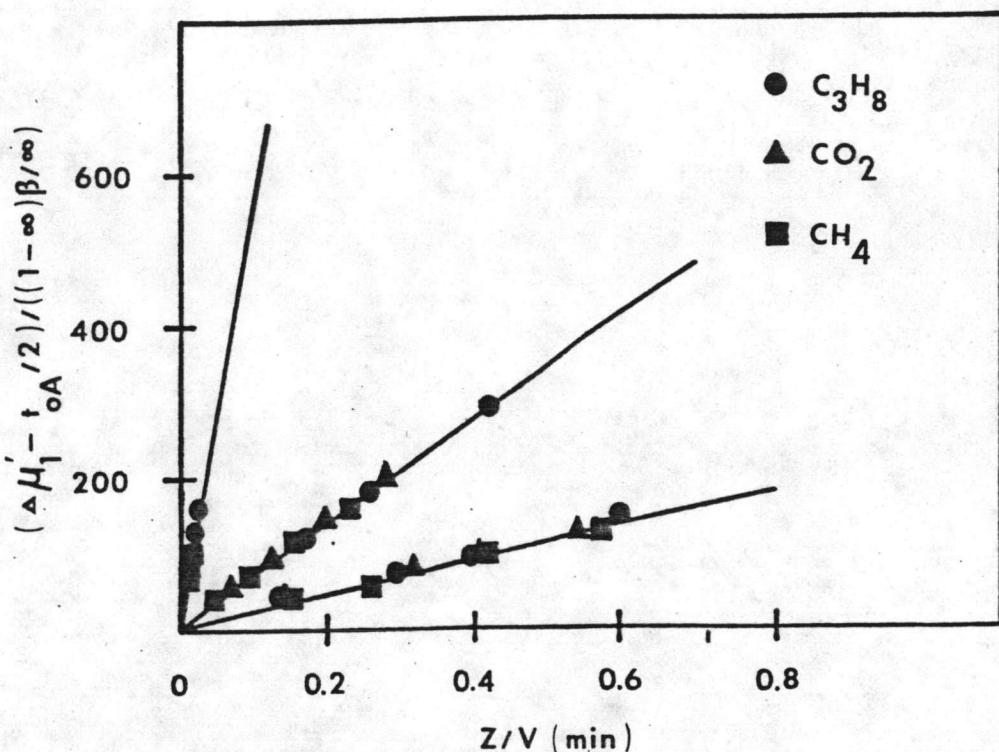
Figure B2 The reduced moment of the square pulses of methane , carbondioxide , and propane at 45 ° C and at a total pressure of 1 bar.

The second central moment of the square pulses of methane , carbondioxide , and propane gives the reduced second central moment and the $1/V^2$ curves as shown in figure B3 , B4 , and B5 respectively.

The y-axis is labeled $(\mu_2 - t_{oA}^2/12)/(2 \times Z/V)$ and the x-axis is labeled $1/V^2 \times 10^4 \ (min/cm)^2$. Legend: R (cm): ● 0.1204, ▲ 0.0940, ■ 0.0674.
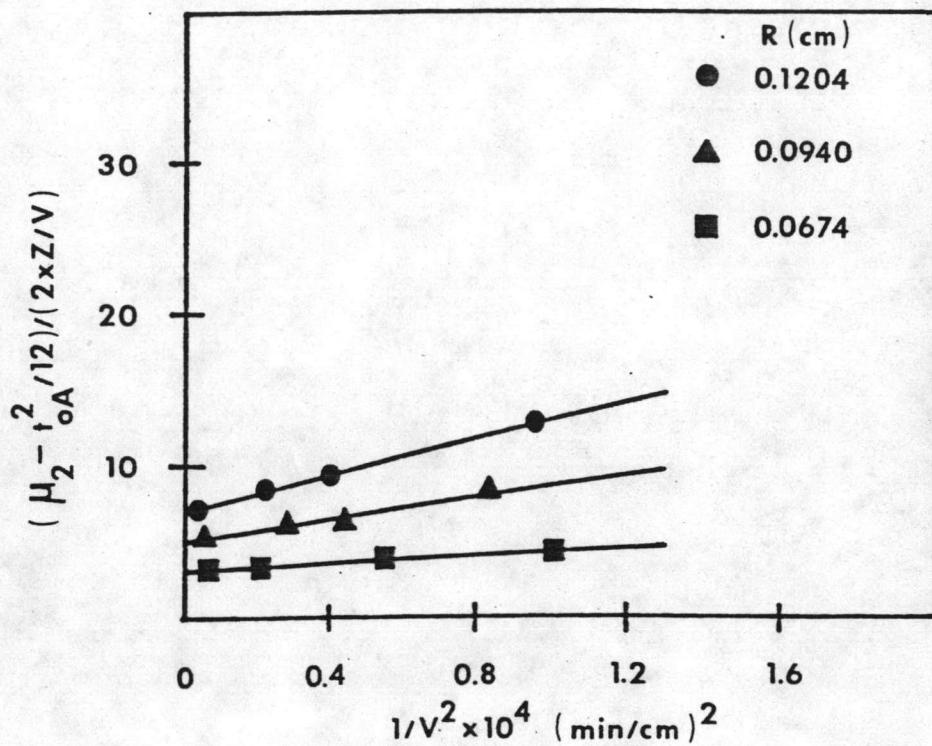
Figure B3   The dependence of reduced second central moments of methane to $1/V^2$.

From the slopes of these curves we can find axial dispersion values for gas flow but only in terms of average values in the range of study and not as a function of flow rate.

The intercepts (b_i) of these curves have a linear relationship with the square of the particle radius as shown in figure B6 , figure B7 , and figure B8 for methane , carbondioxide , and propane respectively.
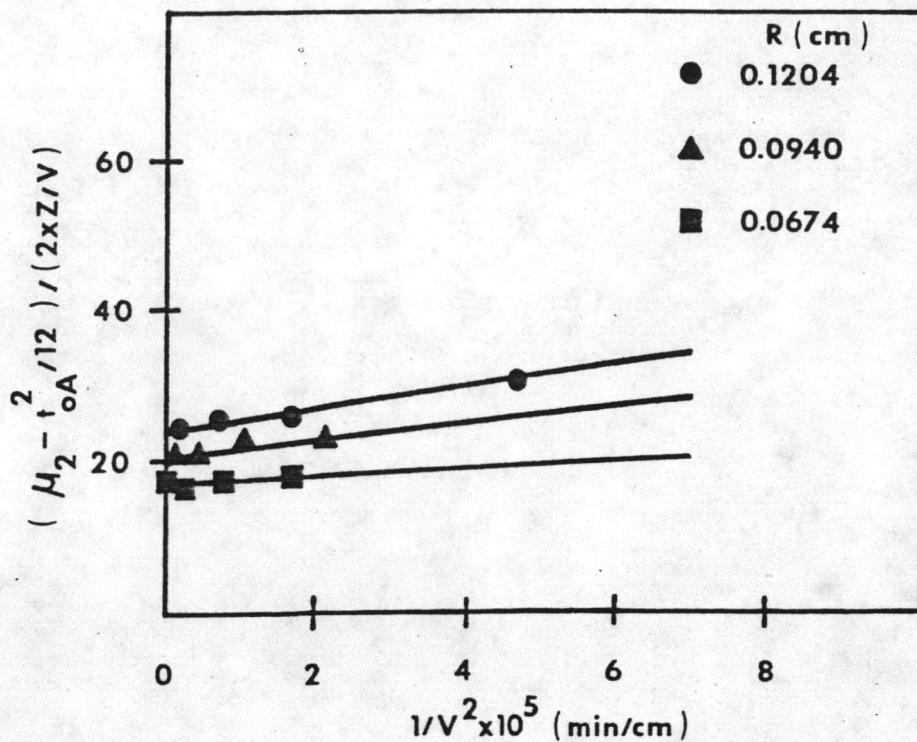
Figure B4   The dependence of the reduced second central moments of carbondioxide to $1/V^2$.

The intercepts of the curve of b_1 and R^2 give the adsorption rate constants for each gas.
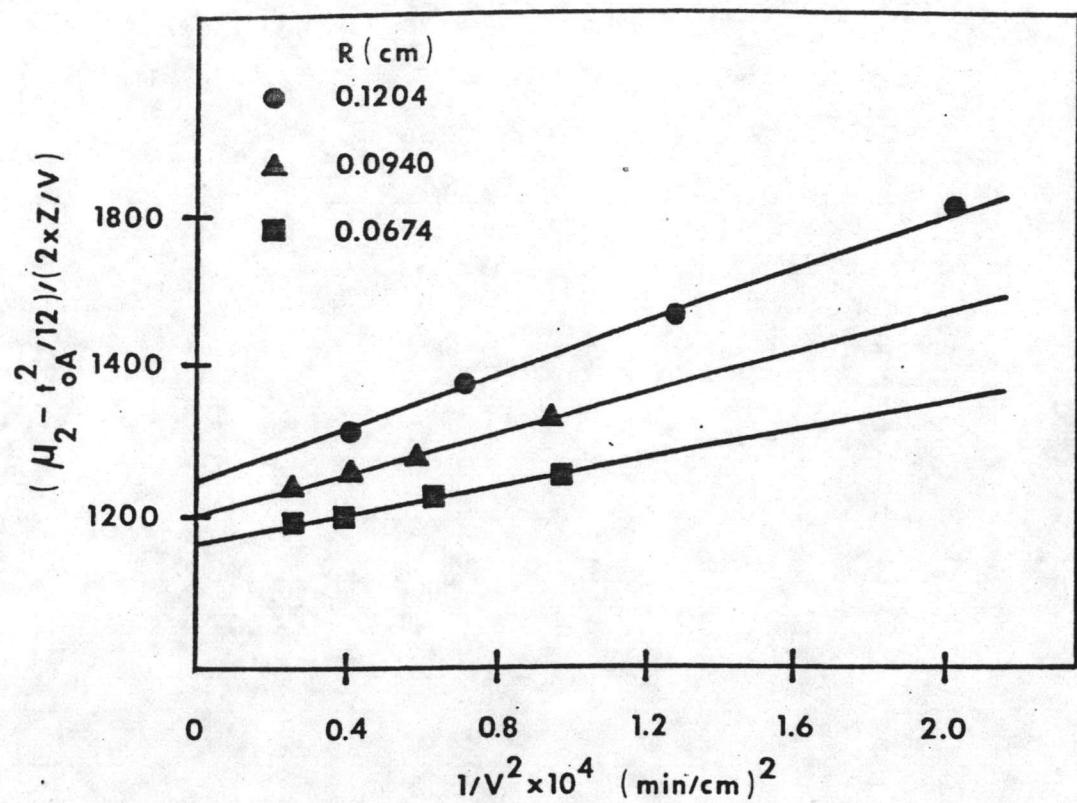
Figure B5 The dependence of the reduced second central moment of propane to $1/V^2$.
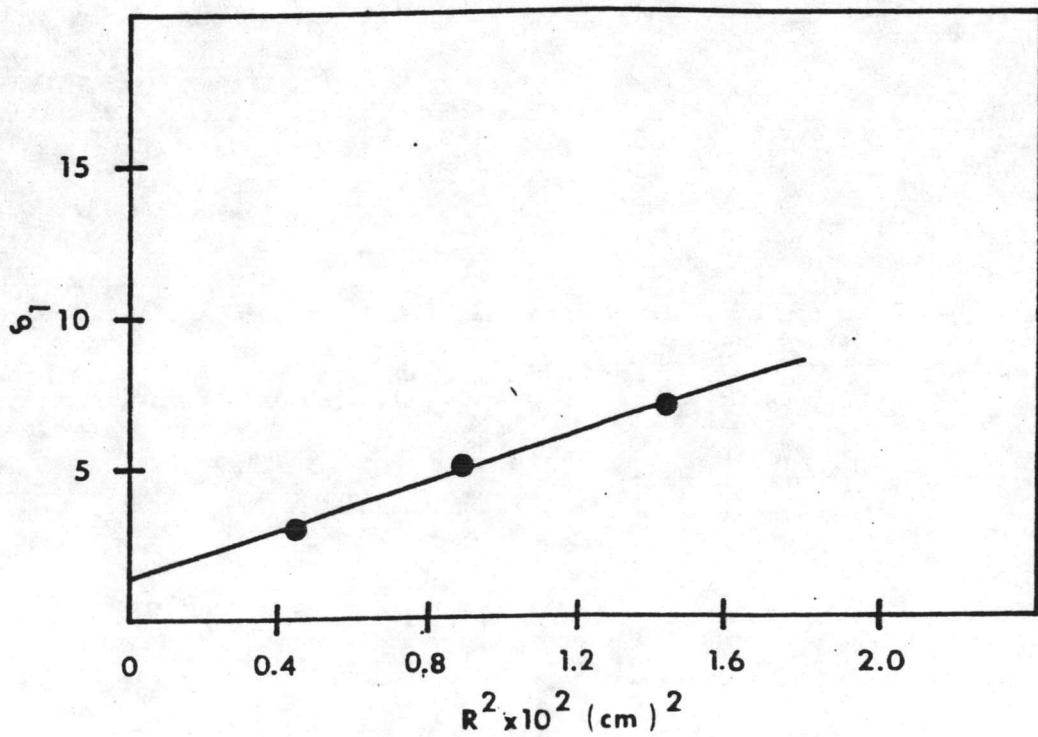
Figure B6 The curve between b_1 and R^2 for methane.
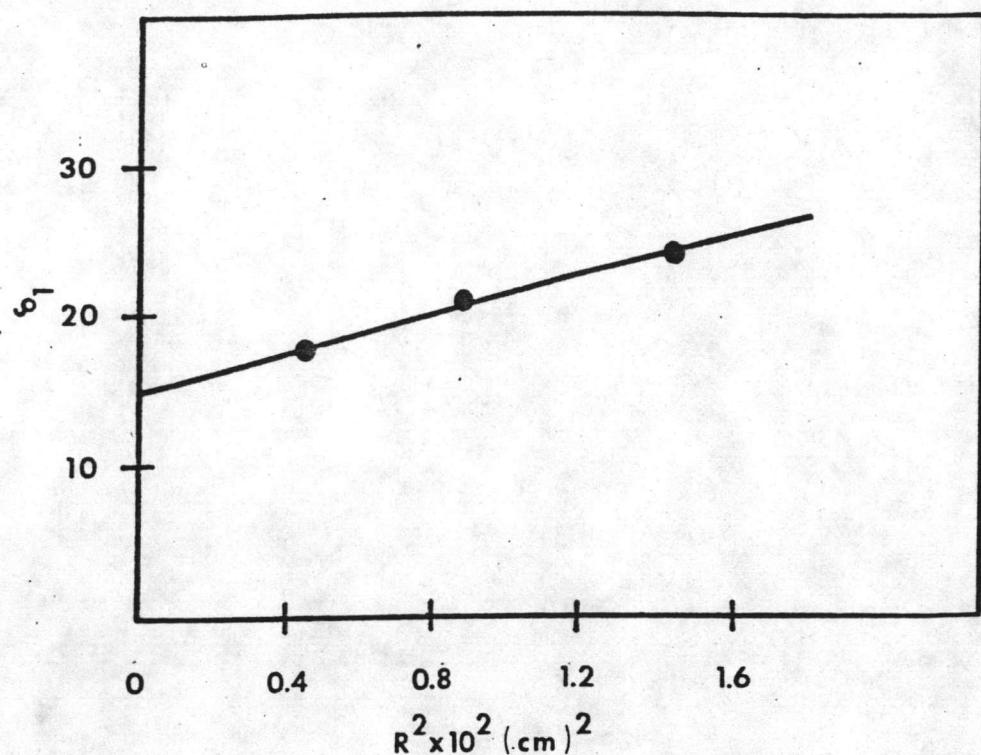
Figure B7 The curve between b_1 and R^2 for carbondioxide.
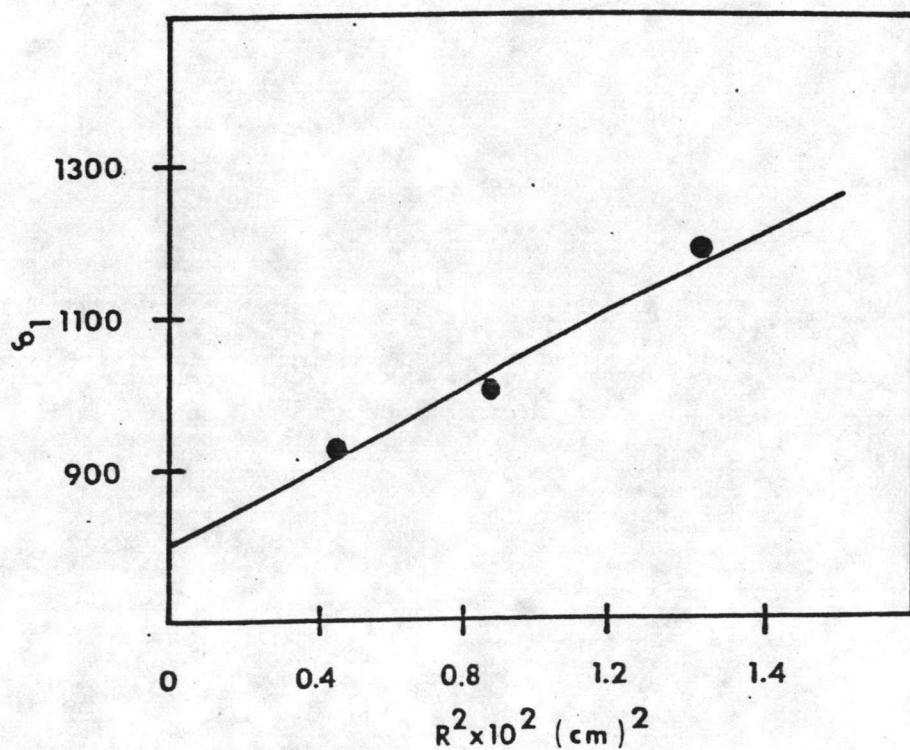
Figure B8 The curve between b_1 and R^2 for propane.

The slopes of the curve between b_1 and R^2 give the intraparticle diffusion coefficients of the gases through the adsorbent particles.

PREDICTION OF C(Z,t)

Previous theoretical treatments that include the resistances of two of the three steps is limited to that of Rosen [16] who considered the combined effects of intraparticle and external diffusion. Later in this thesis solutions are reported for the additional two - resistance cases of intraparticle diffusion - surface adsorption.

With the assumptions shown in chapter 3 the concentration C(Z,t) is determined by the following steps:
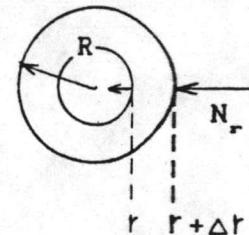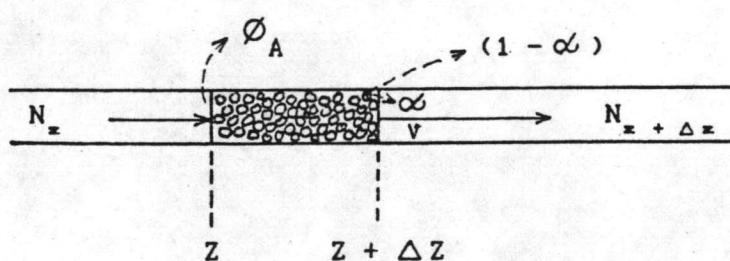
Mass balance in gas phase. (component balance)

$$N_z A \Delta t \Big|_z - N_z A \Delta t \Big|_{z + \Delta z} + v \Delta t A C \Big|_z - v \Delta t A C \Big|_{z + \Delta z} + \alpha A \Delta Z C(t)$$

$$- A \Delta Z C(t + \Delta t) + \langle N_r \rangle 4 \pi R^2 n \Delta t = 0 \qquad ; N_r = \text{average flux}$$

division by $\alpha A \Delta Z \Delta t$ and taking the limit $\Delta Z \to 0$ and $\Delta t \to 0$ gives

$$-\frac{1}{\alpha}\frac{\partial N_z}{\partial z} - \frac{v}{\alpha}\frac{\partial C}{\partial z} - \frac{\partial C}{\partial t} + \langle N_r \rangle 4\pi R^2 N = 0 \qquad ; N = \frac{n}{A\triangle Z}$$

for $N_z = -E_A \dfrac{\partial C}{\partial z}$ then

$$\frac{1}{\alpha} E_A \frac{\partial^2 C}{\partial z^2} - \frac{v}{\alpha}\frac{\partial C}{\partial z} - \frac{\partial C}{\partial t} + \langle N_r \rangle 4\pi R^2 N \frac{3R}{3R} = 0$$

as $\langle N_r \rangle = -D_c\left(\dfrac{\partial C_1}{\partial r}\right)_{r=R}$ and $\dfrac{N 4\pi R^3}{3} = (1-\alpha)$

$$\frac{1}{\alpha} E_A \frac{\partial^2 C}{\partial z^2} - \frac{v}{\alpha}\frac{\partial C}{\partial z} - \frac{\partial C}{\partial t} + \left(-D_c\left(\frac{\partial C_1}{\partial r}\right)_{r=R}\frac{3}{R}\frac{(1-\alpha)}{\alpha}\right) = 0$$

$$\frac{1}{\alpha} E_A \frac{\partial^2 C}{\partial z^2} - v\frac{\partial C}{\partial z} - \frac{\partial C}{\partial t} - \frac{3D_c}{\alpha}\frac{(1-\alpha)}{}\left(\frac{\partial C_1}{\partial r}\right)_{r=R} = 0 \qquad (C.1)$$

Mass balance in the particle gives

$$N_r 4\pi R^2 \triangle t\Big|_{r+\triangle r} - N_r 4\pi R^2 \triangle t\Big|_{r} + \beta 4\pi R^2 \triangle R C_1(t) - \beta 4\pi R^2 \triangle R C_1(t+\triangle t)$$

$$+ \rho_p 4\pi R^2 \triangle R C_{ads}(t) - \rho_p 4\pi R^2 \triangle R C_{ads}(t+\triangle t) = 0$$

division by $4\pi \triangle r \triangle t$ and taking the limit $\triangle t \rightarrow 0$ and $\triangle r \rightarrow 0$ gives

$$\frac{\partial R^2 N_r}{\partial r} - \frac{R^2}{\beta}\frac{\partial C_1}{\partial t} - R^2 \rho_p \frac{\partial C_{ads}}{\partial t} = 0$$

$$2R N_r + R^2 \frac{\partial N_r}{\partial r} - \frac{R^2}{\beta}\frac{\partial C_1}{\partial t} - R^2 \rho_p \frac{\partial C_{ads}}{\partial t} = 0$$

division by βR^2

$$\frac{2 N_r}{\beta R} + \frac{1}{\beta}\frac{\partial N_r}{\partial r} - \frac{\partial C_1}{\partial t} - \frac{\rho_p}{\beta}\frac{\partial C_{ads}}{\partial t} = 0$$

as $N_r = D_c \dfrac{\partial C_1}{\partial r}$

then
$$\frac{D_c}{\beta}\left(\frac{2}{R}\frac{\partial C_1}{\partial r} + \frac{\partial^2 C_1}{\partial r^2}\right) - \frac{\partial C_1}{\partial t} - \frac{\rho_p}{\beta}\frac{\partial C_{ads}}{\partial t} = 0 \quad (C.2)$$

the rate of adsorption , assumed to be linear , may be expressed as

$$\frac{\partial C_{ads}}{\partial t} = k_{ads}(C_1 - C_{ads}/K_A) \quad (C.3)$$

the external diffusion boundary condition may be expressed as

$$D_c \left.\frac{\partial C_1}{\partial r}\right|_{r = R} = k_f (C - C_1) \quad (C.4)$$

the internal diffusion boundary condition may be written as

$$\frac{\partial C_1}{\partial r} = 0 \quad \text{at} \quad r = 0 \quad \text{for} \quad t > 0 \qquad (C.5)$$

and the initial conditions are

$$C = 0 \quad \text{at} \quad Z > 0 \quad \text{for} \quad t = 0 \qquad (C.6)$$

$$C_1 = 0 \quad \text{at} \quad r >= 0 \quad \text{for} \quad t = 0 \qquad (C.7)$$

Conditions (C.6) and (C.7) state that the adsorbent does not contain any adsorbed species as the start of the run. Then condition (C.8) specifies that at the bed inlet the concentration of the adsorbable species is maintained constant , thus

$$C = C_o \quad \text{at} \quad Z = 0 \quad \text{for} \quad t > 0 \qquad (C.8)$$

Recently Masamune and Smith [16] have solved this problem when axial dispersion plays no role ($E_A = 0$) and when the equilibrium adsorption isotherm is linear (Henry's region). They used the mathematical method first developed by Rosen for the case when only intraparticle diffusion is significant as follows

From equation (C.1) with $E_A = 0$ we obtain

$$-\frac{v}{\alpha}\frac{\partial C}{\partial Z} - \frac{\partial C}{\partial t} - \frac{3D_e}{\alpha}\frac{(1-\alpha)}{R}\frac{\partial C_1}{\partial r}\bigg|_{r=R} = 0 \qquad (C.9)$$

$$v \frac{\partial C}{\partial Z} + \alpha \frac{\partial C}{\partial t} + \frac{3D_\varepsilon}{R} \frac{\rho_B}{\rho_P} \left(\frac{\partial C_1}{\partial r} \right)_{r = R} = 0$$

The solution can be simplified by replacing variables Z and t by x and θ in accordance with the expressions

$$x = \frac{Z\alpha}{v} \qquad (C.10)$$

$$\theta = t - \frac{Z\alpha}{v} \qquad (C.11)$$

Then equations (C.9),(C.2),(C.3),(C.6), and (C.7) become

$$\frac{\partial C}{\partial x} + \frac{3 \rho_B D_\varepsilon}{\alpha \rho_P R} \left(\frac{\partial C_1}{\partial r} \right)_{r = R} + \frac{\partial C}{\partial \theta} = 0 \qquad (C.12)$$

$$D_\varepsilon \left(\frac{\partial^2 C_1}{\partial r^2} + \frac{2}{r} \frac{\partial C_1}{\partial r} \right) = \beta \frac{\partial C}{\partial \theta} + \rho_P \frac{\partial C_{ads}}{\partial \theta} \qquad (C.13)$$

$$\frac{\partial C_{ads}}{\partial \theta} = k_{ads} \left(C_1 - C_{ads}/K_A \right) \qquad (C.14)$$

$$C_1 = C = 0, \quad C_{ads} = 0 \quad \text{at} \quad \theta = \frac{Z\alpha}{v} = 0 ; \quad x_0 >= x >= 0 \qquad (C.15)$$

$$C = C_o \quad \text{at} \quad x = 0 \qquad \theta \geq - \frac{Z\alpha}{v} = 0 \qquad (C.16)$$

In equation (C.15) and (C.16) the time interval $Z\alpha/v$ corresponds to the holdup time in the bed and is usually negligible with respect to the time required for finite adsorption.

The solution of equations (C.4),(C.5),(C.12),(C.13), (C.14),(C.15) and (C.16) can be obtained in terms of dimensionless groups, the number of which depends upon the resistances included. When all three resistances are retained , four groups are involved (C.6). The numerical work in evaluating the solution over a range of the four parameters is considerable. Frequently this is not necessary because one or more of the resistances is negligible. For small particles the overall rate is often determined by intraparticle and surface reaction resistances. This case is solved in the next section. Since only three dimensionless parameters are needed , it does not require excessive calculations to evaluate numerically the solution (to obtain C/C_o at Z_o) for a range of values of the parameters.

Intraparticle diffusion and surface adsorption.

The system for this case is described by equation (C.12),(C.13),(C.14),(C.15),(C.16),(C.5) and the form of equation (C.4) which is applicable for negligible external diffusion resistance ; that is

$$C_1 - C = \emptyset \quad \text{at} \quad r = R \qquad \qquad (C.17)$$

The method of solution employed is to apply a double Laplace transform to the variable x and θ . This approach follows that used by Amundson [16] for problems involving diffusion resistances but no surface rate resistance. The symbols used for the transformation are:

$$\mathcal{L}_x [C_1(x,\theta,r)] = \int_0^\infty \exp(-px) \, C_1 \, dx \qquad = f(r,p,\theta) = f_x \qquad (C.18)$$

$$\mathcal{L}_\theta [C_1(x,\theta,r)] = \int_0^\infty \exp(-q\theta) \, C_1 \, d\theta \qquad = f(r,x,q) = f_\theta \qquad (C.19)$$

$$\mathcal{L}_{x\theta}[C_1(x,\theta,r)] = \int_0^\infty \exp(-(px+q\theta))C_1 dxd\theta = f(r,p,q) = f_{x\theta} \qquad (C.20)$$

$$\mathcal{L}_x [C_{ads}(x,\theta,r)] = \int_0^\infty \exp(-px) \, C_{ads} \, dx \qquad = g(r,p,\theta) = g_x \qquad (C.21)$$

$$\mathcal{L}_\theta [C_{ads}(x,\theta,r)] = \int_0^\infty \exp(-qx) \, C_{ads} \, d\theta \qquad = g(r,x,q) = g_\theta \qquad (C.22)$$

$$\mathcal{L}_{x\theta}[C_{ads}(x,\theta,r)] = \int_0^\infty \exp(-(px+qx))C_{ads} dxd\theta = g(r,p,q) = g_{x\theta} \qquad (C.23)$$

and for the interparticle gas concentration C

$$\mathcal{L}_x [C(x,\theta)] = \int_0^\infty \exp(-px)Cdx \qquad = F(p,\theta) = F_x \qquad (C.24)$$

$$\mathcal{L}_\theta [C(x,\theta)] = \int_0^\infty \exp(-qx)Cd\theta \qquad = F(x,q) = F_\theta \qquad (C.25)$$

$$\mathcal{L}_{x\theta}[C(x,\theta)] = \int_0^\infty \exp(-(px+q\theta)Cdxd\theta \qquad = F(p,q) = F_{x\theta} \qquad (C.26)$$

Using the relation for the transform of the first derivative, and applying the initial condition one obtains

$$\mathcal{L}_x \left[\mathcal{L}_\theta \left(\frac{dC_1}{d\theta} \right) \right] = \mathcal{L}_x \ [[C_1 \exp(-q\theta)]_0^\infty + q \int_0^\infty C_1 \exp(-q\theta) d\theta] = \mathcal{L}_x \{qf_\theta\} = qf_{x\theta}$$

(C.27)

Similarly for the variables C_1 and C, when one utilizes the boundary conditions of equation (C.16)

$$\mathcal{L}_x \left[\mathcal{L}_\theta \left(\frac{\partial C_{ads}}{\partial \theta} \right) \right] = qg_{x\theta}$$

(C.28)

$$\mathcal{L}_\theta \left[\mathcal{L}_x \left(\frac{\partial C}{\partial x} \right) \right] = \mathcal{L}_\theta [C_o + pF_x] = \frac{-C_\theta}{q} + pF_{x\theta}$$

(3.29)

Now application of the double transform produce to equations (C.12),(C.13),(C.14), and (C.17) reduces the problem to the solution of the following set of ordinary differential and algebraic equations:

$$\frac{-C_o}{q} + pF_{x\theta} + C_1 \left(\frac{df_{x\theta}}{dr} \right)_{r=R} = 0$$

(C.30)

$$\text{where} \quad C_1 = \frac{3 \rho \ D_c}{\rho_p \alpha R}$$

$$D_e\left[\frac{d^2 f_{x\theta}}{dr^2} + \frac{2}{r}\frac{df_{x\theta}}{dr}\right] = q\,(\beta f_{x\theta} + \rho_p q_{x\theta}) \qquad (C.31)$$

$$qg_{x\theta} = k_{ads}\,(f_{x\theta} - q_{x\theta}/K_A)$$

$$= \overrightarrow{\lambda} f_{x\theta} - \overleftarrow{\mu} q_{x\theta} \qquad ; \quad \overrightarrow{\lambda} = k_{ads}$$

$$\overleftarrow{\mu} = k_{ads}/K_A \qquad (C.32)$$

$$(F_{x0})_{r=R} = (f_{x0})_{r=R} \qquad (C.33)$$

combination of equation (C.31) and (C.32) gives the following equation in f_{x0} :

$$\frac{d^2 f_{x\theta}}{dr^2} + \frac{2}{r}\frac{df_{x\theta}}{dr} - \frac{q[\,\beta + \rho_p\overrightarrow{\lambda}/(q+\overleftarrow{\mu})\,]f_{x\theta}}{D_e} = 0$$

Since β is negligible with respect to $(\overrightarrow{\lambda}\rho_p)/(q+\overleftarrow{\mu})$, the equation may be written as

$$\frac{d^2 f_{x\theta}}{dr^2} + \frac{2}{r}\frac{df_{x\theta}}{dr} - \rho_p\frac{\overrightarrow{\lambda}}{D_e}\,\frac{q}{q+\overleftarrow{\mu}}\,f_{x\theta} = 0 \qquad (C.34)$$

The general solution of equation (C.34) using Bessel's function differential form is

$$f_{x\theta} = \frac{C_2}{r}\sin\left[r\sqrt{-\rho_p\frac{\overrightarrow{\lambda}}{D_e}\,\frac{q}{q+\overleftarrow{\mu}}}\right] + \frac{C_3}{r}\cos\left[r\sqrt{-\rho_p\frac{\overrightarrow{\lambda}}{D_e}\,\frac{q}{q+\overleftarrow{\mu}}}\right]$$

However the constant C_3 must vanish since $f_{x\theta}$ should be finite at $r = 0$. Hence the solution reduces to

$$f_{x\theta} = \frac{C_2}{r} \sin\left(\frac{rhW(q)}{R}\right) \tag{C.35}$$

where $W(q)$ and h are defined by the expressions

$$W(q) = i\sqrt{\frac{q}{q + \mu}}$$

$$h = R\sqrt{\frac{\lambda \rho_p}{D_c}}$$

The constant C_2 can be evaluated from equation (C.30) and (C.33). The result is

$$C_2 = \frac{C_o R}{q} \frac{1}{\sin[hW(q)]} \frac{1}{p + (C1/R)\{hW(q)\cot[hW(q)] - 1\}} \tag{C.36}$$

Then the solution for $f_{x\theta}$ becomes

$$f_{x\theta} = \frac{RC_o}{rq} \frac{\sin[(rhW(q)/R)]}{\sin[hW(q)]} \frac{1}{p + (C_1/R)\{hW(q)\cot[hW(q)] - 1\}} \tag{C.37}$$

The next step is to use the inverse transform to obtain f_θ from equation (C.37). Then equation (C.9) is

transformed with respect to θ , obtaining an ordinary differential equation in dF_θ/dx and involving df_θ/dr . This may be solved for F_θ . Then the inverse transform gives the required solution for C as a fuction of x and θ . [Equation (C.25)] Carrying out these steps one can apply the inverse transform relationship

$$\mathcal{L}^{-1}[\ 1\ /\ (p + a)] = e^{-ax} \tag{C.38}$$

in equation (C.37) to obtain

$$f_\theta = \frac{RC_o}{q}\ \frac{\sin[(rhW(q))/R]}{\sin[hW(q)]}\ \exp[-(C_1/R)x\{hW(q)\cot[hW(q)]-1\}] \tag{C.39}$$

Now transforming equation (C.9) with respect to θ one gets

$$\frac{dF_\theta}{dx} + C_1\left(\frac{df_\theta}{dr}\right)_{r\ =\ R} = 0 \tag{C.40}$$

The term $(df_\theta/dr)_{r\ =\ R}$ can be evaluated from equation (C.39). If this is done , and the result integrated , we obtained

$$F_\theta = \frac{C_o}{q} \exp\ [-\ (C_1/R)x\{hW(q)\cot[hW(q)]-1\}] \tag{C.41}$$

Now the solution may formally be written as the inverse transform of equation (C.41) ; that is

$$C(x,\theta) = \frac{1}{2\pi i} \lim_{\beta \to \infty} \left[\int_{r-i\beta}^{r+i\beta} e^{q\theta} F_\theta \, dq \right] \qquad (C.42)$$

The function F_θ has a single pole at $q = 0$ and an infinite number of unessential singularities on the negative side of the real axis. Hence it is not practical to evaluate the integral in equation (C.42) by the method of summing the residues. However by substituting $q/\overleftarrow{\mu} = i\beta/\overleftarrow{\mu} = y^2$, it is possible to transform the integral into a real, improper form. In this manner equation (3.42) can be written in terms of the integration parameter y (and substitute every terms to the initial form) as follows :

$$\frac{C(Z,t)}{C_o} = \frac{1}{2} + \frac{2}{\pi} \int_0^\infty \frac{1}{y} \exp[A_1(y)] \sin[A_2(y)] \, dy \qquad (C.43)$$

$$A_1(y) = -3D[w_1 + E(w_1 + w_2)]/[(1 + Ew_1)^2 + (Ew_2)^2] \qquad (C.44)$$

$$A_2(y) = D\{A\gamma y^2 - [3w_2/[(1 + Ew_1)^2 + (Ew_2)^2]]\} \qquad (C.45)$$

$$w_1 = [\phi_1 \sin(2\phi_1) + \phi_2 \sinh(2\phi_2)]/[\cosh(2\phi_2) - \cos(2\phi_1)] - 1 \qquad (C.46)$$

$$w_2 = [\phi_2 \sin(2\phi_1) + \phi_1 \sinh(2\phi_2)]/[\cosh(2\phi_2) - \cos(2\phi_1)] \qquad (C.47)$$

$$\phi_1 = -\sqrt{Ay^2/[2(y^4 + 1)(\sqrt{y^4 + 1} + y^2)]} \qquad (C.48)$$

$$\emptyset_2 = \sqrt{Ay^2 / [2(y^4 + 1)(\sqrt{y^4 + 1} - y^2)]} \qquad (C.49)$$

In these equations $\mathcal{T}$ is a normalized time

$$\mathcal{T} = t/t_o \qquad (C.50)$$

where t_o is the time necessary for saturation of the adsorbent under conditions where there is no résistance at all. It is given by

$$t_o = \frac{1 - \alpha}{\alpha} \rho_p K_A \frac{Z}{v} \qquad (C.51)$$

The dimensionless parameters D,E, and A are defined as follows :

$$D = \frac{D_c}{R^2} \frac{1 - \alpha}{\alpha} \frac{Z}{v} \qquad (C.52)$$

$$E = \frac{D_c}{k_f R} \qquad (C.53)$$

$$A = \frac{R^2}{D_c} k_{ads} \rho_p \qquad (C.54)$$

They contain the rate constants which describe external diffusion , internal diffusion , and adsorption rate ,

When the rate constants D_c , k_f and k_{ads} are known , it is possible to calculate by means of equations (C.43) to (C.54) the $C = C(t, Z = const.)$ curve , point by point , for an adsorber bed characterized by the values of Z , α , ρ_p , R , and for a specific value of the gas velocity , v.

$C(Z,t)$ can be predicted by using equations 3.10 to 3.21 and the parameters obtained in this work such as the adsorption rate constants , the intraparticle diffusion coefficients , the mass transfer coefficients , and the binary diffusion coefficient. The program used based on equation 3.10 to 3.21 is as follows

```
DEFDBL A-H,J-Z
CLS
KA=1053.0756
RADS=637.6373
DC=.3327
KF=57.1277
DP=.9673
R=.12108
Z=61.7234
V=7249.5243
ALFA=.8630
A=(R^2)*RADS*DP/DC
E=DC/(KF*R)
D=(DC^/(R^2))*((1-ALFA)/ALFA)*Z/V
T0=((1-ALFA)/ALFA)*DP*KA*Z/V
LOCATE 5,15 : PRINT "A =";A
LOCATE 6,15 : PRINT "E =";E
LOCATE 7,15 : PRINT "D =";D
LOCATE 8,15 : PRINT "T0=";T0
FOR I = 2 TO 16 STEP 2
IK=0
CC=0
TAO=I/10
T=TAO*T0
FOR J = .00000000000001 TO .4 STEP .00000000000001
IK=IK+1
Y=J
FAI2=((A*Y^2)/(2*((Y^4)+1)*(((Y^4)+1)^(0.5)-Y^2)))^(0.5)
FAI1=-((A*Y^2)/(2*((Y^4)+1)*(((Y^4)+1)^(0.5)+Y^2)))^(0.5)
S1=(EXP(2*FAI2)-EXP(-2*FAI2))/2
CO2=(EXP(2*FAI2)+EXP(-2*FAI2))/2
IF (CO2-COS(2*FAI1)) = 0 GOTO 5
W2=(FAI2*SIN(2*FAI1)+FAI1*S1)/(CO2-COS(2*FAI1))
W1=((FAI1*SIN(2*FAI1)+FAI2*S1)/(CO2-COS(2*FAI1)))-1
A2=D*(A*TAO*Y^2-(3*W2/((1+E*W1)^2+(E*W2)^2)))
A1=-3*D*(W1+E*(W1^2+W2^2))/((1+E*W1)^2+(E*W2)^2)
C=(1/Y)*(EXP(A1))*SIN(A2)
IF (INT(IK/2))*2 = IK GOTO 10
5 CC=CC+(.00000000000001/3)*4*C : GOTO 20
10 CC=CC+(.00000000000001/3)*2*C
20 LOCATE 15,15 : PRINT "TAO =";TAO
LOCATE 16,15 : PRINT "TIME =";T
LOCATE 17,15 : PRINT "C     =";C
LOCATE 18,15 : PRINT "C(Z,T) =";CC*14/22+.5
NEXT J
LOCATE 20,15 : PRINT "C(Z,T) =";CC*14/22+.5
NEXT I
END
```

ADSORBENT COLUMN REGENERATION CONDITIONS

The regeneration conditions used in this study for
the adsorption column are compared to regenerating conditions
mentioned in the literature are presented in figure D1.
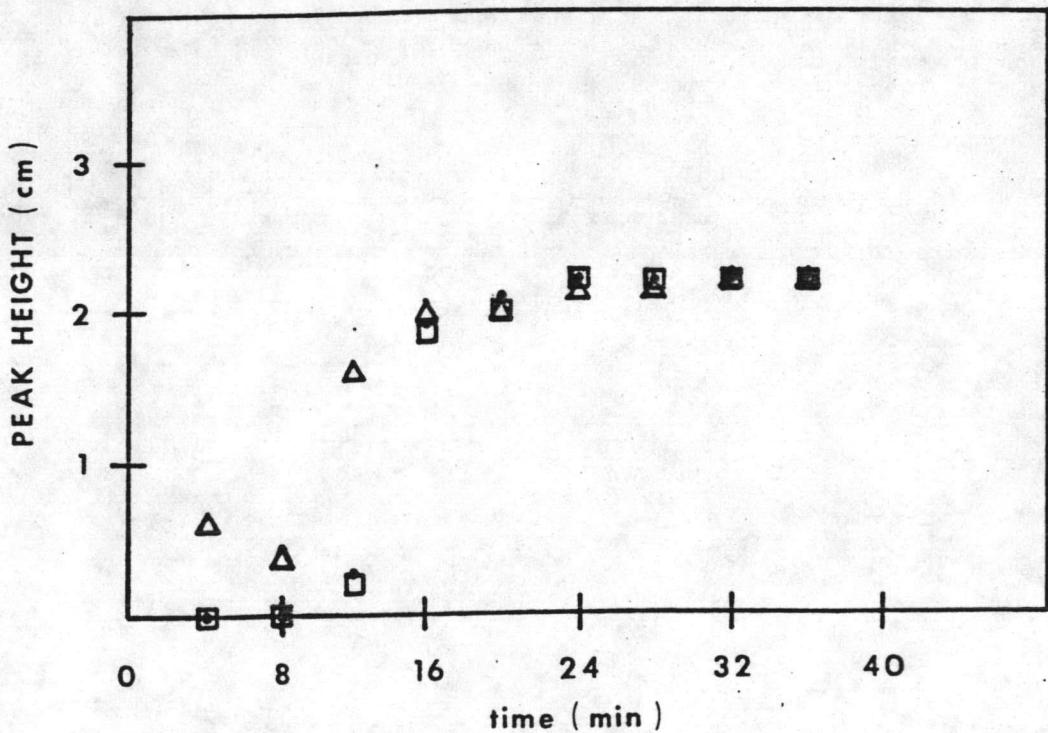
Figure D1 The breakthrough curve for the adsorption
of methane after the following regeneration conditions
• at 300 ° C , 0.3 torrs , 6 hours (condition used in
this work)

□ at 400 ° C , 760 torrs , 3 hours , and helium flow 0.5

cc/sec [Chihara , Suzuki , Carbon , Pergamon press Ltd , Vol. 17

, 1979 , pp 339 - 343].

$\triangle$ at 300 ° C , 0.3 torrs , 3 hours

We see that the regeneration conditions used in this work have the same characteristic curve for the adsorption of methane. Thus we can use these regeneration conditions for regenerating adsorbents in each run.

APPENDIX E

DETERMINATION OF PARTICLE SIZES

The particles were crushed and sieved with 20 - 30 mesh screens. The particle sizes were determined by a microscope with a spectromicrometer using Ferret's method as shown in figure E1. The size distributions of the particles were found to have the same shape as shown in figure E2. The average diameter used are the surface mean diameters which have the following relationship

$$\text{surface mean diameter} = d_{pan} = \left(\frac{\sum n d_p^2}{\sum n} \right)^{1/2}$$
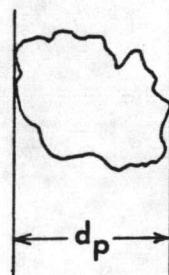
Figure E1 Ferret's diameter , must be the longest dimension along the line parallel to the base of the field of view.

The surface mean obtained were 0.1348 , 0.1880 , and 0.2407 cm.
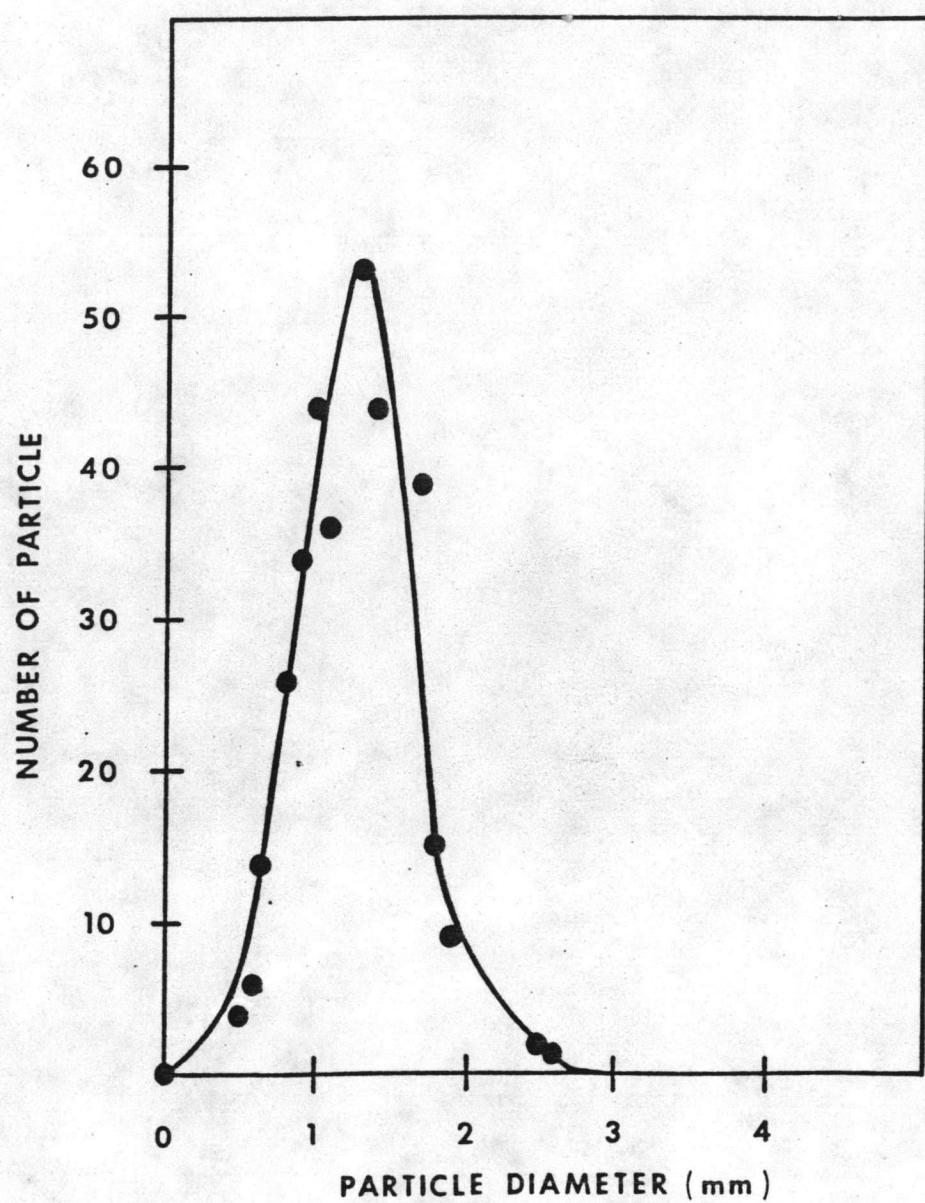
Figure E2   Size distribution of particle with size average of 0.1348 cm.
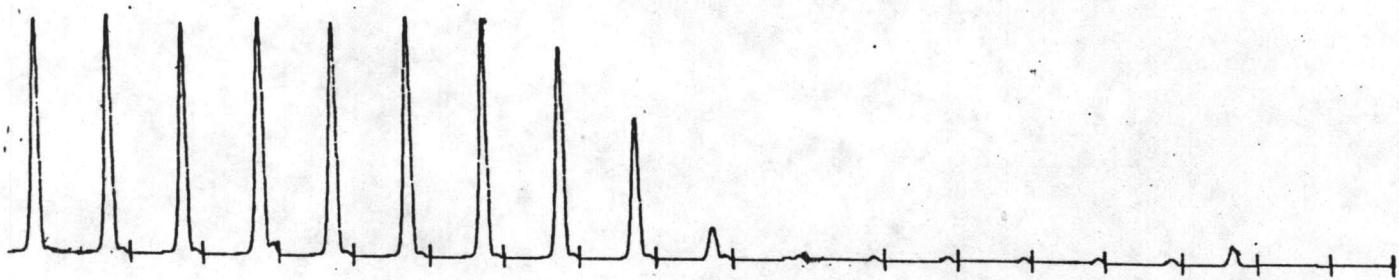
Figure F1   The chromatographic peaks of methane adsorbed   on

molecular   sieve   carbon − 5A   at   45 ° C with a flow rate   of

16.9358 cc/min and a concentration of 2.4 percent methane.
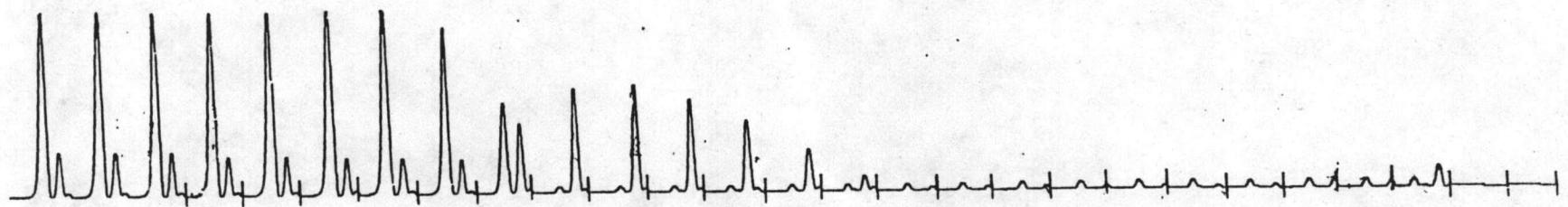
Figure F2 The chromatographic peaks of a mixture of methane and carbondioxide (0.9 % methane and 99.1 % carbondioxide) at a total pressure of 0.5 bar and at 45 ° C with a flow rate of 14.4620 cc/min.
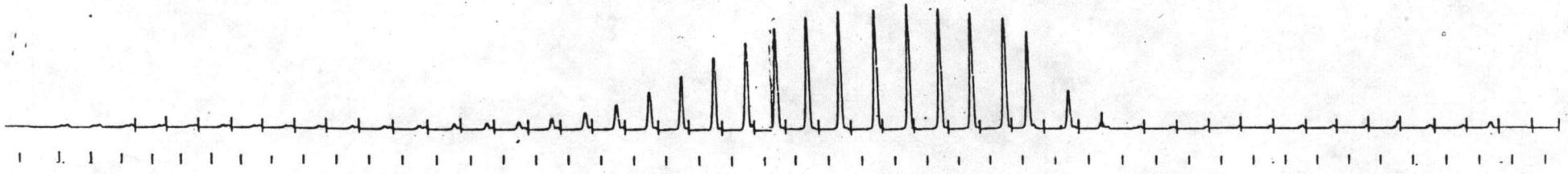
Figure   F3   The chromatographic peaks of an output   of   a

ten   minutes square pulse of methane at a concentration   of

2.4 percent and at a temperature of 45 $^\circ$ C with a flow   rate

of   9.7726 cc/min.

APPENDIX G

SAMPLE CALCULATION OF A CHROMATOGRAPHIC CURVE

The output of a ten minutes square pulse chromatographic peaks of propane at a Z/v of 0.0125 and at a concentration of 0.88 % is presented in table G1

TABLE G1

The output of one chromatographic peak for propane.

Z/v = 0.0125   0.88 % propane 45° C   R = 0.1204 cm

time (min)	mole(propane)/cc	time (min)	mole/cc
1.1666	0	24.3333	2.1122×10^{-4}
2.3333	0	25.5000	1.9949×10^{-4}
3.5000	0	26.6667	1.8776×10^{-4}
4.6667	3.1291×10^{-4}	27.8333	1.7603×10^{-4}
5.8333	1.5906×10^{-3}	29.0000	1.6430×10^{-4}
7	2.1643×10^{-3}	30.1666	1.5257×10^{-4}
8.1666	2.2947×10^{-3}	31.3333	1.4084×10^{-4}
9.3333	2.2947×10^{-3}	32.5000	1.2911×10^{-4}
10.5000	1.9818×10^{-3}	33.6667	1.1738×10^{-4}
11.6667	1.7992×10^{-3}	34.8333	1.0565×10^{-4}
13.8333	1.1473×10^{-3}	36.0000	0.9392×10^{-4}
15.0000	7.0405×10^{-4}	37.1666	0.8219×10^{-4}

16.1666	5.2152×10^{-4}	38.3333	0.7046×10^{-4}
17.3333	4.1722×10^{-4}	39.5000	0.5873×10^{-4}
18.5000	3.7158×10^{-4}	40.6667	0.4700×10^{-4}
19.6667	3.2594×10^{-4}	41.8333	0.3527×10^{-4}
20.8333	2.8030×10^{-4}	43.0000	0.2354×10^{-4}
22	2.3468×10^{-4}	44.1666	0.1181×10^{-4}
23.1666	2.2295×10^{-4}	45.3333	0.0000

The first absolute and second central moment calculated by a BASICA program in appendix B for propane at different flow rates are tabulated in table G2

TABLE G2

First absolute and second central moment (R=0.1204)

	Z/V			
	0.0125	0.0166	0.0221	0.0228
μ_1'	11.8421	13.5267	16.6098	19.1993
$(\mu_1')_{inert}$	0.0136	0.0180	0.0240	0.0313
$\dfrac{(\Delta \mu_1' - t_o A/2)}{(\beta(1-\alpha)/\alpha)}$	78.9422	98.3665	133.9399	163.7919
$1/V^2 \times 10^7$	0.4101	0.7233	1.2820	2.1771
μ_2	38.8931	53.2944	75.8168	113.4609
$(\mu_2 - t_o A/12)/(2Z/V)$	1222.3920	1354.2500	1526.7760	1825.1320

A plot of the reduced moments VS. Z/V is a straight line

through the origin as shown in figure B2. The slopes of these curves are equal to $\rho_p K_A / \beta$. Thus we can find the equilibrium constants (K_A) of methane , propane , and carbondioxide from these slopes as shown in table G2.

TABLE G3

The equilibrium constants

($\rho_p = 0.9673$, $\beta = 0.1819$)   gas

	methane	propane	carbondioxide
slope	208.8565	5600.0000	632.5717
K_A	39.2753	1053.0756	118.9546

A plot of a reduced second central moment VS. $1/V^2$ are shown in figure B3 , B4 , and B5 for methane , carbondioxide , and propane respectively. The slopes of these curve equal to

$E_A (1 + \delta_o)^2 / \alpha$

From equation 3.34 we have

$$\delta_o = [(1-\alpha) \beta / \alpha] [1 + (\rho_p / \beta) K_A]$$
$$= 104.7683$$

From this δ_o we can find E_A from the slopes as follows The slope of the curve between $1/V^2$ and reduced second central moment of propane adsorbed on 0.2408 cm MSC-5A is equal to 352.9412×10^6. Thus the axial dispersion coefficient has a value of 2.0917×10^6 cm^2/min.

Binary molecular diffusivity (D) calculated by [Bird , Stewart , and Lightfoot , " Transport phenomena" , John Wiley , New York (1960)]

$$D_{AB} = 0.0018583 \sqrt{T^3(1/M_A + 1/M_B)} / P\sigma_{AB}^2 \Omega_{D,AB}$$

at T = 318 K

P = 1 atm

argon = A

methane , ethane , and carbondioxide = B

	argon	methane	carbondioxide	propane
σ °A	3.418	3.822	3.996	5.061
ϵ_A/K °K	124.000	137.000	190.000	254.000
$\sigma_{AB} = (\sigma_A + \sigma_B)/2$		3.620	3.707	4.240
$\epsilon_{AB} = \sqrt{\epsilon_A \epsilon_B}$		130.338	153.493	177.471
KT/ϵ_{AB}		2.440	2.072	1.792
		1.007	1.062	1.118
D_{AB} cm²/min		14.160	9.468	6.876

From equation 3.46 we have

$$k_f R = D_{AB}$$

Thus we can find k_f from this equation as follows

k_f of propane passing through a packed column of 0.2408 cm particles has a value of 57.1277 cm^2/min.

The intercept of the curves of reduced second central moment VS. $1/V^2$ equal to b_1. A plot of b_1 VS. R^2 be a straight line curves as shown in figure B6 , B7 , B8 for methane , carbondioxide , and propane respectively. The intercepts of these curves equal to b_2 in equation 3.42. b_2 of methane , carbondioxide , and propane are 1.40 , 14.9 , and 800 respectively. Thus we can find the adsorption rate constants from

$$b_2 = (\beta(1-\alpha)/\alpha)(\rho_D/\beta)K_A^2/k_{ads}$$

The adsorption rate constants are shown in table VIII. The slopes of the lines in figure B6 , B7 , B8 are equal to $(b_1 + b_2)/R^2$. Since k_f and K_A are known , b_2 can be determined and with these slopes to establish values of b_1. Then D_c is obtained from equation 3.43 shown in table IX.

The prediction of C(Z,t) using a turbo basic program.

C(Z,t) can be predicted using a turbobasic program as shown in appendix C. The calculation time is about 3 hours for each point of the breakthrough curve. This program was run on the IBM-PC-XT with an 8087 math processor chip. The results of the prediction of the breakthrough curve for

propane at a velocity of 3202.3956 cm/min are as follows

A = 26.85631729042161

E = 4.838646362213779E-002

D = 0.2210550460457212

T0 = 9.804664293870282

TAO = 0.2

TIME = 1.960932858774056

$C(Z,t)/C_o = 0$

TAO(reduced time) and $C(Z,T)/C_o$ are summarized in table G3.

TABLE G4

TAO	C(Z,T)
0.2	0
0.4	0.0000000000000087
0.6	0.0000000000001327
0.8	0.0000000000231490
1.0	0.4823467210890045
1.2	0.9999876310000000
1.4	1.0000000000000000
1.6	1.0000000000000000

The breakthrough curve of the data from table G4 are shown
in figure 5.6. The parameters obtained from this program are
of the same order as those obtained by P.Schneider and J.M.
Smith as shown in table G4

TABLE G5

Hydrcarbon	D	E	A
ethane	3.24	2.39×10^{-3}	340.00
propane	68.1	3.19×10^{-3}	24.1
n-butane	8.1	6.36×10^{-3}	1468.0

$Z = 30.1$, $R = 0.5, 0.11, 0.5$ mm for ethane , propane , n-butane respectively

The constants D , E , and A are calculated from the equations (3.19) , (3.20) , and (3.21) respectively.

AUTOBIOGRAPHY

Tanetr satrawaha was born on June 3 , 1962 in Roi-Et , Thailand. He attended Watbenjamabopitr High School in Bangkok and graduated in 1981. He resieved his Bachelor of Science Degree in chemistry from Chiangmai University , Thailand , in March 1985. He continued his Master's study at Chulalongkorn University in 1988. He was granted the degree in May 1989.