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## APPENDICES

### Appendix A Natural Gas Composition

**Table A1** The composition of natural gas collected from the upstream of dehydration unit of Gas Separation Plant Unit 1 (Rayong), PTT Public Company Limited (PTTPLC), Receive date: 06/12/02

<b>Composition</b>	<b>Molecular Weight</b>	<b>%mol or %vol</b>
Nitrogen, N <sub>2</sub>	28	2.11
Methane, CH <sub>4</sub>	16	78.95
Ethane, C <sub>2</sub> H <sub>6</sub>	30	9.76
Propane, C <sub>3</sub> H <sub>8</sub>	44	5.31
i-Butane, C <sub>4</sub> H <sub>10</sub>	58	1.27
n-Butane, C <sub>4</sub> H <sub>10</sub>	58	1.15
Pentane+, C <sub>5</sub> +	72	0.84
CO <sub>2</sub>	44	0.61
Average molecular weight	<b><u>20.764</u></b>	100.00

## Appendix B Adsorbent Information

**Table B1** The general information of three adsorbents, Zeolite Type 4A with pellet size 1/16", 1/8" and Silica gel

Typical Properties	MolSiv 4A 1/16" pellets	MolSiv 4A 1/8" pellet	Silica gel
Chemical Formula	$\text{Na}_{12}[(\text{AlO}_2)_{12}(\text{SiO}_2)_{12}] \cdot x\text{H}_2\text{O}$		$\text{SiO}_2 \cdot \text{H}_2\text{O}$
Nominal Pore Diameter	4 Angstroms	4 Angstroms	NA
Bulk Density	41 lb/ft <sup>3</sup>	41 lb/ft <sup>3</sup>	46.4 lb/ft <sup>3</sup>
Particle Diameter	0.0575 in. to 0.0775 in.	0.1150 in. to 0.01350 in.	8 mesh or 0.1120 in.
Surface Area	NA	NA	340 m <sup>2</sup> /g
Heat of Adsorption (max.)	1800	1800	NA
Equilibrium H <sub>2</sub> O Capacity*	22%wt	22%wt	NA

\* Lbs H<sub>2</sub>O/100 lbs activated adsorbent at 17.5 mmHg, 25°C

### Appendix C Adsorbent Layout

**Table C1** Adsorber layout of the multi-layer adsorber used in the adsorption study

Adsorber Layout	Adsorbent Type	Height (cm)	Weight (g)
	Silica gel	0.4	2.9643
	MolSiv (Zeolite) Type 4A with pellet size 1/8"	5.5	33.0121
	MolSiv (zeolite) Type 4A with pellet size 1/16"	2.9	20.6566
	Ceramic ball	*Inert material used as an adsorbent support	

Adsorber volume: 75 ml

## Appendix D Definition of Relative Humidity

Relative humidity,  $H_R$  is defined as the ratio of the partial pressure of the vapor to the vapor pressure of the liquid at the gas temperature. It is usually expressed on a percentage basis, so 100% humidity means saturated gas and 0% humidity means vapor-free gas, McCabe, (1993).

$$\%H_R = \frac{100 \times P_A}{P_A^0}$$

at gas condition of 25 °C, 1 bar,  $P_A^0 = 0.03132$  bar or 3131.753741 mPa, McCabe, (1993). It was defined that the saturation partial pressure is equal to the vapor pressure of water at the gas temperature.

**Table D1** Humidity conversion at gas condition of 25 °C and 1 atm

$H_R$ %	$P_A$ (bar) = $H_R \cdot P_A^0 / 100$	$P_A$ kPa	$P_A$ mPa	mol fraction, $y_A$		ppm(mole) or ppm(V)
				= $P_A / P_T$	% mol	
0.1	0.00003	0.00313	3.13175	0.00003	0.003	31.318
0.2	0.00006	0.00626	6.26351	0.00006	0.006	62.635
0.3	0.00009	0.00940	9.39526	0.00009	0.009	93.953
0.4	0.00013	0.01253	12.52701	0.00013	0.013	125.270
0.5	0.00016	0.01566	15.65877	0.00016	0.016	156.588
0.6	0.00019	0.01879	18.79052	0.00019	0.019	187.905
0.7	0.00022	0.02192	21.92228	0.00022	0.022	219.223
0.8	0.00025	0.02505	25.05403	0.00025	0.025	250.540
0.9	0.00028	0.02819	28.18578	0.00028	0.028	281.858
1	0.00031	0.03132	31.31754	0.00031	0.031	313.175
2	0.00063	0.06264	62.63507	0.00063	0.063	626.351
3	0.00094	0.09395	93.95261	0.00094	0.094	939.526
4	0.00125	0.12527	125.27015	0.00125	0.125	1252.701
5	0.00157	0.15659	156.58769	0.00157	0.157	1565.877
6	0.00188	0.18791	187.90522	0.00188	0.188	1879.052
7	0.00219	0.21922	219.22276	0.00219	0.219	2192.228
8	0.00251	0.25054	250.54030	0.00251	0.251	2505.403
9	0.00282	0.28186	281.85784	0.00282	0.282	2818.578
10	0.00313	0.31318	313.17537	0.00313	0.313	3131.754
11	0.00344	0.34449	344.49291	0.00344	0.344	3444.929

Continued

Table D1 (Continue)

H <sub>R</sub> %	P <sub>A</sub> (bar) = H <sub>R</sub> *P <sub>A</sub> <sup>o</sup> /100	P <sub>A</sub> kPa	P <sub>A</sub> mPa	mol fraction, y <sub>A</sub>		ppm(mole) or ppm(V)
				=P <sub>A</sub> /P <sub>T</sub>	% mol	
12	0.00376	0.37581	375.81045	0.00376	0.376	3758.104
13	0.00407	0.40713	407.12799	0.00407	0.407	4071.280
14	0.00438	0.43845	438.44552	0.00438	0.438	4384.455
15	0.00470	0.46976	469.76306	0.00470	0.470	4697.631
16	0.00501	0.50108	501.08060	0.00501	0.501	5010.806
17	0.00532	0.53240	532.39814	0.00532	0.532	5323.981
18	0.00564	0.56372	563.71567	0.00564	0.564	5637.157
19	0.00595	0.59503	595.03321	0.00595	0.595	5950.332
20	0.00626	0.62635	626.35075	0.00626	0.626	6263.507
21	0.00658	0.65767	657.66829	0.00658	0.658	6576.683
22	0.00689	0.68899	688.98582	0.00689	0.689	6889.858
23	0.00720	0.72030	720.30336	0.00720	0.720	7203.034
24	0.00752	0.75162	751.62090	0.00752	0.752	7516.209
25	0.00783	0.78294	782.93844	0.00783	0.783	7829.384
26	0.00814	0.81426	814.25597	0.00814	0.814	8142.560
27	0.00846	0.84557	845.57351	0.00846	0.846	8455.735
28	0.00877	0.87689	876.89105	0.00877	0.877	8768.910
29	0.00908	0.90821	908.20859	0.00908	0.908	9082.086
30	0.00940	0.93953	939.52612	0.00940	0.940	9395.261
31	0.00971	0.97084	970.84366	0.00971	0.971	9708.437
32	0.01002	1.00216	1002.16120	0.01002	1.002	10021.612
33	0.01033	1.03348	1033.47873	0.01033	1.033	10334.787
34	0.01065	1.06480	1064.79627	0.01065	1.065	10647.963
35	0.01096	1.09611	1096.11381	0.01096	1.096	10961.138
36	0.01127	1.12743	1127.43135	0.01127	1.127	11274.313
37	0.01159	1.15875	1158.74888	0.01159	1.159	11587.489
38	0.01190	1.19007	1190.06642	0.01190	1.190	11900.664
39	0.01221	1.22138	1221.38396	0.01221	1.221	12213.840
40	0.01253	1.25270	1252.70150	0.01253	1.253	12527.015
41	0.01284	1.28402	1284.01903	0.01284	1.284	12840.190
42	0.01315	1.31534	1315.33657	0.01315	1.315	13153.366
43	0.01347	1.34665	1346.65411	0.01347	1.347	13466.541
44	0.01378	1.37797	1377.97165	0.01378	1.378	13779.716
45	0.01409	1.40929	1409.28918	0.01409	1.409	14092.892
46	0.01441	1.44061	1440.60672	0.01441	1.441	14406.067
47	0.01472	1.47192	1471.92426	0.01472	1.472	14719.243
48	0.01503	1.50324	1503.24180	0.01503	1.503	15032.418
49	0.01535	1.53456	1534.55933	0.01535	1.535	15345.593
50	0.01566	1.56588	1565.87687	0.01566	1.566	15658.769

Continued

Table D1 (Continue)

H <sub>R</sub> %	P <sub>A</sub> (bar) = H <sub>R</sub> *P <sub>A</sub> <sup>o</sup> /100	P <sub>A</sub> kPa	P <sub>A</sub> mPa	mol fraction, y <sub>A</sub>		ppm(mole) or ppm(V)
				=P <sub>A</sub> /P <sub>T</sub>	% mol	
51	0.01597	1.59719	1597.19441	0.01597	1.597	15971.944
52	0.01629	1.62851	1628.51195	0.01629	1.629	16285.119
53	0.01660	1.65983	1659.82948	0.01660	1.660	16598.295
54	0.01691	1.69115	1691.14702	0.01691	1.691	16911.470
55	0.01722	1.72246	1722.46456	0.01722	1.722	17224.646
56	0.01754	1.75378	1753.78210	0.01754	1.754	17537.821
57	0.01785	1.78510	1785.09963	0.01785	1.785	17850.996
58	0.01816	1.81642	1816.41717	0.01816	1.816	18164.172
59	0.01848	1.84773	1847.73471	0.01848	1.848	18477.347
60	0.01879	1.87905	1879.05224	0.01879	1.879	18790.522
61	0.01910	1.91037	1910.36978	0.01910	1.910	19103.698
62	0.01942	1.94169	1941.68732	0.01942	1.942	19416.873
63	0.01973	1.97300	1973.00486	0.01973	1.973	19730.049
64	0.02004	2.00432	2004.32239	0.02004	2.004	20043.224
65	0.02036	2.03564	2035.63993	0.02036	2.036	20356.399
66	0.02067	2.06696	2066.95747	0.02067	2.067	20669.575
67	0.02098	2.09828	2098.27501	0.02098	2.098	20982.750
68	0.02130	2.12959	2129.59254	0.02130	2.130	21295.925
69	0.02161	2.16091	2160.91008	0.02161	2.161	21609.101
70	0.02192	2.19223	2192.22762	0.02192	2.192	21922.276
71	0.02224	2.22355	2223.54516	0.02224	2.224	22235.452
72	0.02255	2.25486	2254.86269	0.02255	2.255	22548.627
73	0.02286	2.28618	2286.18023	0.02286	2.286	22861.802
74	0.02317	2.31750	2317.49777	0.02317	2.317	23174.978
75	0.02349	2.34882	2348.81531	0.02349	2.349	23488.153
76	0.02380	2.38013	2380.13284	0.02380	2.380	23801.328
77	0.02411	2.41145	2411.45038	0.02411	2.411	24114.504
78	0.02443	2.44277	2442.76792	0.02443	2.443	24427.679
79	0.02474	2.47409	2474.08546	0.02474	2.474	24740.855
80	0.02505	2.50540	2505.40299	0.02505	2.505	25054.030
81	0.02537	2.53672	2536.72053	0.02537	2.537	25367.205
82	0.02568	2.56804	2568.03807	0.02568	2.568	25680.381
83	0.02599	2.59936	2599.35561	0.02599	2.599	25993.556
84	0.02631	2.63067	2630.67314	0.02631	2.631	26306.731
85	0.02662	2.66199	2661.99068	0.02662	2.662	26619.907
86	0.02693	2.69331	2693.30822	0.02693	2.693	26933.082
87	0.02725	2.72463	2724.62576	0.02725	2.725	27246.258
88	0.02756	2.75594	2755.94329	0.02756	2.756	27559.433
89	0.02787	2.78726	2787.26083	0.02787	2.787	27872.608

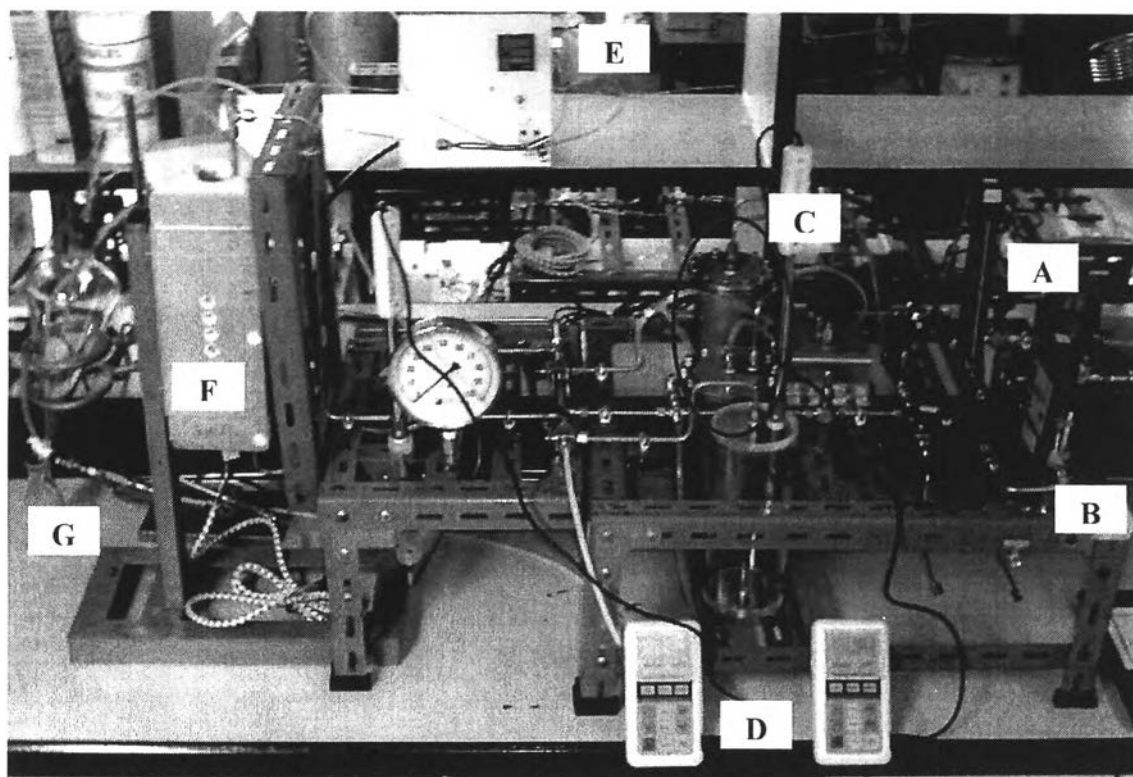
Continued



**Table D1 (Continue)**

H <sub>R</sub> %	P <sub>A</sub> (bar) = H <sub>R</sub> *P <sub>A</sub> <sup>o</sup> /100	P <sub>A</sub> kPa	P <sub>A</sub> mPa	mol fraction, y <sub>A</sub>		ppm(mole) or ppm(V)
				=P <sub>A</sub> /P <sub>T</sub>	% mol	
90	0.02819	2.81858	2818.57837	0.02819	2.819	28185.784
91	0.02850	2.84990	2849.89590	0.02850	2.850	28498.959
92	0.02881	2.88121	2881.21344	0.02881	2.881	28812.134
93	0.02913	2.91253	2912.53098	0.02913	2.913	29125.310
94	0.02944	2.94385	2943.84852	0.02944	2.944	29438.485
95	0.02975	2.97517	2975.16605	0.02975	2.975	29751.661
96	0.03006	3.00648	3006.48359	0.03006	3.006	30064.836
97	0.03038	3.03780	3037.80113	0.03038	3.038	30378.011
98	0.03069	3.06912	3069.11867	0.03069	3.069	30691.187
99	0.03100	3.10044	3100.43620	0.03100	3.100	31004.362
100	0.03132	3.13175	3131.75374	0.03132	3.132	31317.537

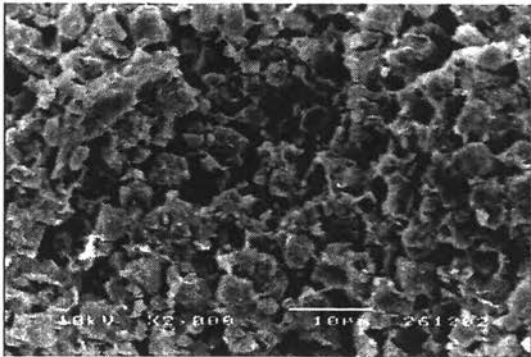
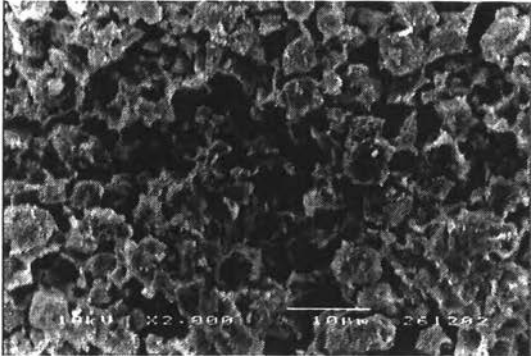
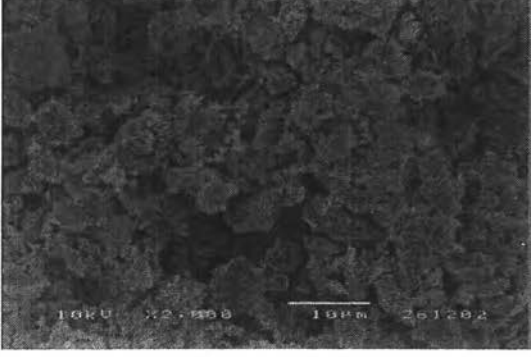
## Appendix E Experimental Setup



**Figure E1** Experimental Setup: A = Flow meter, B = Mass flow controller, C = Humidifier, D = Humidifier analyzer, E = Temperature controller, F = Electric heater, and G = Separator.

## Appendix F Morphology of Fresh Adsorbents

The morphology of fresh adsorbent was observed by Scanning Electron Microscopoe (SEM) as shown below.

Adsorbent type	x 3,500
4ADG 1/8" (4A ZEOLITE)	 <p>SEM image showing the morphology of 4ADG 1/8" (4A ZEOLITE) at x3,500 magnification. The image displays a highly porous, irregular, and interconnected network of particles, characteristic of zeolite-based adsorbents. A scale bar at the bottom indicates 1000 units, and technical parameters like 10KV X2,000 and 100um 261202 are visible.</p>
4ADG 1/16" (4A ZEOLITE)	 <p>SEM image showing the morphology of 4ADG 1/16" (4A ZEOLITE) at x3,500 magnification. The image displays a highly porous, irregular, and interconnected network of particles, characteristic of zeolite-based adsorbents. A scale bar at the bottom indicates 1000 units, and technical parameters like 10KV X2,000 and 100um 261202 are visible.</p>
LCA-94 SILICA GEL	 <p>SEM image showing the morphology of LCA-94 SILICA GEL at x3,500 magnification. The image displays a highly porous, irregular, and interconnected network of particles, characteristic of silica gel-based adsorbents. A scale bar at the bottom indicates 1000 units, and technical parameters like 10KV X2,000 and 100um 261202 are visible.</p>

## Appendix G Simulation Program

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C#####
C
C   PROGRAM BREAKTHROUGH CURVE PREDICTION
C
C   THIS PROGRAM WAS DEVELOPED TO CALCULATE THE CONCENTRATION OF WATER IN
C   THE NATURAL GAS LEAVING FROM THE ADSORBER WITH RESPECT TO TIME AND
C   LENGTH. AND ALSO THE ADSORPTION CAPACITY WAS EVALUATED. THE METHOD OF
C   LINE (MOL) COMBINED WITH THE RUNGE-KUTTA 4th ORDER WAS APPLIED TO
C   SOLVE THE SET OF MASS TRANSFER AND ADSORPTION EQUATION.
C
C#####

      IMPLICIT NONE
      DOUBLE PRECISION C0,C,q,dt,KC,Kq,time
      INTEGER i,j,imax,jmax,n
      PARAMETER(imax=90,jmax=5000)
      DIMENSION C(imax,jmax),q(imax,jmax)
      DIMENSION KC(4,imax,jmax),Kq(4,imax,jmax)

C*****INITIAL CONDITION*****

      dt = 0.01
      C0 = 7.672460743E-04      !inlet concentration (mol/l) at 60%RH
      time=0
      j=1                      !at time = 0

      C(1,j)=C0

      OPEN(5,file='Accul(kel 0).dat')

      DO i=2,imax

         C(i,j)=0
         q(i,j)=0

      END DO

      OPEN(1,file='data1.dat')

      DO i=1,imax
         WRITE(1,101)time,i,j,C(i,j),q(i,j)
      END DO

      Call RK4(j,C,q,imax,jmax,KC,Kq,dt)

      GOTO 20

10 OPEN(2,FILE='DATA2.DAT')

      DO i=2,imax

         READ(2,102)time,C(i,1),q(i,1),(KC(n,i,1),n=1,4)
1         ,(Kq(n,i,1),n=1,4)

      END DO

```

```

20 DO j=2,jmax
      DO i=2,imax
            C(1,j)=C0
            C(i,j)=C(i,j-1)+(dt/6)*(KC(1,i,j-1)+2*KC(2,i,j-1)
1          +2*KC(3,i,j-1)+KC(4,i,j-1))

            q(i,j)=q(i,j-1)+(dt/6)*(Kq(1,i,j-1)+2*Kq(2,i,j-1)
1          +2*Kq(3,i,j-1)+Kq(4,i,j-1))

      END DO

      Call RK4(j,C,q,imax,jmax,KC,Kq,dt)

END DO

C*****RECORD RESULTS*****

DO j=1,jmax
      time=time+dt      !sec

END DO

CLOSE(2)
OPEN(2,file='data2.dat')
DO i=2,imax

      WRITE(2,102)time,C(i,jmax),q(i,jmax),(KC(n,i,jmax),n=1,4)
1      ,(Kq(n,i,jmax),n=1,4)

      WRITE(5,102)time,C(i,jmax),q(i,jmax)

END DO

CLOSE(2)

C*****CONTINUE CALCULATION BY CHECKING AND RETURNING LOOP*****

IF(time.LT.251999) THEN
GOTO 10
ELSE
GOTO 999
END IF

C*****FORMAT FOR INPUT AND OUTPUT STATEMENTS*****

101 FORMAT(F13.3,I3,I6,2E15.9,8E15.9)
102 FORMAT(F13.3,2E15.9,8E15.9)

999  STOP

      END

C*****

```

C=-----

```

SUBROUTINE RK4 (j, C, q, imax, jmax, KC, Kq, dt)

IMPLICIT NONE
DOUBLE PRECISION CC, qq, C, q, dC_dt, dq_dt, dt, KC, Kq
INTEGER i, j, imax, jmax
DIMENSION C(imax, jmax), q(imax, jmax), dC_dt(imax, jmax)
DIMENSION dq_dt(imax, jmax), KC(4, imax, jmax), Kq(4, imax, jmax)
DIMENSION CC(imax, jmax), qq(imax, jmax)

DO i=1, imax

    CC(i, j)=C(i, j)
    qq(i, j)=q(i, j)

END DO

Call ODEs_EQ(j, imax, jmax, CC, qq, dC_dt, dq_dt)

DO i=2, imax

    KC(1, i, j)=dC_dt(i, j)
    Kq(1, i, j)=dq_dt(i, j)
    CC(i, j)=CC(i, j)+(dt/2)*KC(1, i, j)
    qq(i, j)=qq(i, j)+(dt/2)*Kq(1, i, j)

END DO

    Call ODEs_EQ(j, imax, jmax, CC, qq, dC_dt, dq_dt)

DO i=2, imax

    KC(2, i, j)=dC_dt(i, j)
    Kq(2, i, j)=dq_dt(i, j)

    CC(i, j)=CC(i, j)+(dt/2)*KC(2, i, j)
    qq(i, j)=qq(i, j)+(dt/2)*Kq(2, i, j)

END DO

    Call ODEs_EQ(j, imax, jmax, CC, qq, dC_dt, dq_dt)

DO i=2, imax

    KC(3, i, j)=dC_dt(i, j)
    Kq(3, i, j)=dq_dt(i, j)

    CC(i, j)=CC(i, j)+(dt)*KC(3, i, j)
    qq(i, j)=qq(i, j)+(dt)*Kq(3, i, j)

END DO

    Call ODEs_EQ(j, imax, jmax, CC, qq, dC_dt, dq_dt)

```

```

DO i=2,imax

    KC(4,i,j)=dC_dt(i,j)
    Kq(4,i,j)=dq_dt(i,j)

END DO

Return

End

C-----
SUBROUTINE ODES_EQ(j,imax,jmax,c,q,dC_dt,dq_dt)

IMPLICIT NONE
DOUBLE PRECISION c,q,dC_dt,dz,L,d2C_dz2,DL1,v1,e1,dq_dt
DOUBLE PRECISION dC_dz,qstar,a1,b1,k1,db_A,a2
INTEGER i,j,imax,jmax
DIMENSION C(imax,jmax),q(imax,jmax),dC_dt(imax,jmax)
DIMENSION d2C_dz2(imax,jmax),dC_dz(imax,jmax),qstar(imax,jmax)
DIMENSION dq_dt(imax,jmax)

C .....Define Parameter.....

L =8.8                ! Total bed length
dz = L/(imax-2)      ! Step size for length

C .....Parameter of Adsorber.....

db_A=0.74522533545    ! Bulk density of adsorbent
v1= 0.487112708      ! Effective interstitial velocity through
DL1=0.046391158      ! Effective axial dispersion through
e1=0.520578990       ! Effective void fraction

C .....Adsorption Isotherm Constant Parameter.....

a1 =2.465497336E+06   ! For Langmuir-Isotherm
b1 =1.263717318E+05
k1 =1.004023607E-04   ! Effective overall mass transfer coefficient

a2 =2.855735511E+04   ! For Linear-Isotherm

j=j

DO i=2,imax

    If(i.LT.imax) then

        If(C(i,j).GE.6.652814423E-04) then

            qstar(i,j)=a2*C(i,j)

        Else

            qstar(i,j)=(a1*C(i,j))/(1+b1*C(i,j))

        END If

    END DO

```

```

dq_dt(i,j)=k1*(qstar(i,j)-q(i,j))
d2C_dz2(i,j)=(1/(dz**2))*(C(i+1,j)-2*C(i,j)+C(i-1,j))
dC_dz(i,j)=(1/(2*dz))*(C(i+1,j)-C(i-1,j))
dC_dt(i,j)=DL1*d2C_dz2(i,j)-v1*dC_dz(i,j)-((1-e1)/e1)
1 *dq_dt(i,j)*db_A/1.8
Else
qstar(imax,j)=qstar(imax-1,j)
dq_dt(imax,j)=dq_dt(imax-1,j)
d2C_dz2(imax,j)=0
dC_dz(imax,j)=0
dC_dt(imax,j)=dC_dt(imax-1,j)
End If
END DO
Return
End

```



## APPENDIX H

### Kelvin Equation

The capillary condensation within the pore of adsorbent can be explained by Kelvin equation (Ruthven, 1984).

$$\frac{P}{P_s} = \exp\left(\frac{-2\sigma V_m \cos \theta}{rRT}\right) \quad (\text{H-1})$$

where

$\frac{P}{P_s}$  = relative pressure of vapor at equilibrium

$\sigma$  = surface tension of the liquid adsorbed, (N/m)

$V_m$  = molar volume of the liquid adsorbed, (m<sup>3</sup>/mole)

$\theta$  = contact angle (for capillary condensation  $\theta = 0$ )

$R$  = gas constant, (8.314 J/mole.K)

$T$  = adsorption temperature, (K)

$r$  = pore radius of adsorbent, (m)

## CURRICULUM VITAE

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