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APPENDICES

Appendix A Calculation and Sample of Calculation

A1 Calculation of Sulfur Concentration

A1.1 Calibration of Sulfur Compounds

From

$$n_i * RMR_i = A_i$$

$$n_{std} * RMR_{std} = A_{std}$$

$$\text{So, } RMR_i = \frac{A_i * n_{std}(RMR_{std})}{A_{std} * n_i} \qquad \text{(A1.1.1)}$$

A1.2 Concentration of Sulfur Compounds in the Simulated Fuels

$$Y_i = \frac{A_i / RMR_i}{\sum_{i=1}^{n} [A_i / RMR_i]} \qquad \text{(A1.2.1)}$$

A_i = Peak area of component *i*

n_i = Concentration of component *i* (weight basis)

A_{std} = Peak area of standard component

n_{std} = Concentration of standard component (weight basis)

RMR_i = Respond factor of component *i*

RMR_{std} = Respond factor of standard component

Y_i = Concentration of component *i* from calibration

Respond factor of component i (RMR_i)

RMR of 3-methylthiophene = 0.6714

RMR of benzothiophene = 0.7720

RMR of dibenzothiophene = 0.8174

Respond factor of standard component (RMR_{std})

RMR of isooctane = 1

RMR of decane = 1

Example: Adsorption of 3-methylthiophene in isooctan on NaX zeolite at room temperature

A1.2.1 Data from Table

Initial Concentration

Peak area of 3-MT#1 ($A_{3\text{-}MT}$#1) = 47592

Peak area of 3-MT#2 ($A_{3\text{-}MT}$#2) = 48493

Peak area of isooctane#1 (A_{std}#1) = 67643958

Peak area of isooctane#2 (A_{std}#2) = 68625420

Concentration at 61.5 min of adsorption time

Peak area of 3-MT#1 ($A_{3\text{-}MT}$#1) = 3106

Peak area of 3-MT#2 ($A_{3\text{-}MT}$#2) = 3120

Peak area of isooctane#1 (A_{std}#1) = 68616031

Peak area of isooctane#2 (A_{std}#2) = 69840243

A1.2.2 To Calculate the Initial Concentration of 3-MT in Isooctane

For the initial concentration of 3-MT#1

$$Y_{3\text{-}MT}\#1 = \frac{(47592/0.6714)}{(47592/0.6714) + (67643958/1)}$$

$$= 0.0010468121 * 10^6$$

$$= 1046.8121 \text{ ppmw}$$

For the initial concentration of 3-MT#2

$$Y_{3\text{-}MT}\#2 = \frac{(48493/0.6714)}{(48493/0.67144) + (68625420/1)}$$

$$= 0.0010513707 * 10^6$$

$$= 1051.3707 \text{ ppmw}$$

Average of $Y_{3\text{-MT}} = (1046.8121+1051.3707)/2$

$$= 1049.0914 \text{ ppmw}$$

A1.2.3 To Calculate the Concentration of 3-MT in Isooctane at 61. 5 min of Adsorption Time

For the equilibrium concentration of 3-MT#1

$$Y_{3\text{-MT}}\#1 = \frac{(3106/0.6714)}{(3106/0.6714) + (68616031/1)}$$

$$= 0.0000674164 * 10^6$$

$$= 67.4164 \text{ ppmw}$$

For the equilibrium concentration of 3-MT#2

$$Y_{3\text{-MT}}\#2 = \frac{(3120/0.6714)}{(3120/0.6714) + (69840243/1)}$$

$$= 0.0000665332* 10^6$$

$$= 66.5332 \text{ ppmw}$$

Average of $Y_{3\text{-MT}} = (67.4164 + 66.5332)/2$

$$= 66.9748 \text{ ppmw}$$

A1.2.4 To Convert Adsorption Time to Treated Volume

Volumetric flow rate = 0.5 $cm^3 min^{-1}$

Total bed weight = 0.5040 g

Adsorption time = 61.5 min

$$\text{Treated Volume} = \frac{61.5 *0.5}{0.5040} = 61.0119 \text{ } cm^3 g^{-1} \text{ adsorbent}$$

A1.2.4 To Convert the Concentration at t to the Ratio of Initial Concentration

$$C(t)/\,C(i) = \frac{66.9748}{1049.091} = 0.0638$$

A2 Calculation the Adsorption Capacity of Zeolite

$$q_{breakthrough} = \left(\frac{v}{m_{adsorbent}}\right)\left(\frac{\rho_{fuel} X_i}{MW_{sulfur}}\right)\int_0^t \left[1 - \frac{C(t)}{C_i}\right] dt \qquad \text{(A2.1)}$$

V = the volumetric flow rate of feed stream ($cm^3\ min^{-1}$),

ρ_{fuel} = the fuel density at room temperature ($g\ cm^{-3}$),

X_i = the total sulfur fraction (by weight) in the feed

C_i = the total sulfur concentration in the feed (ppmw)

$m_{adsorbent}$ = the weight of adsorbent bed (g)

MW_{sulfur} = the molecular weight pf sulfur

$C\,(t)$ = the effluent total sulfur concentration (ppmw) at any time t (min)

$\frac{v}{m_{adsorbent}}\int_0^t \left[1 - \frac{C(t)}{C(i)}\right] dt$ = area above the breakthrough curve

A2.1 Calculation the Breakthrough and Saturation Capacity of Zeolite

Example: Breakthrough and saturation capacity of NaX in adsorption 3-methylthiophene from isooctane

$\rho_{isooctane} = 0.692\ g\ cm^{-3}$

Xi = 1049.0914/1000000 = 0.0010490914

C_i = 1049.0914 ppmw

$m_{adsorbent}$ = 0.5040 g

$MW_{3\text{-}MT}$ = 98.1624

Tabel A1 The data for calculation the adsorption capacity of zeolite

Position	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	Area under Breakthrough Curve (iim 0→ Treated Vol.)
Breakthrough point (5 ppmw)	18.6232	0.0054
Saturation point (C(t)/C(i) = 0.95)	342.1797	153.4078

Note: The treated volume at breakthrough and saturation point were taken by interpolation the data of the breakthrough curve.

The area under the breakthrough curve was taken from the calculation of Sigma Plot software.

Then, for breakthrough point

$$\frac{v}{m_{adsorbent}}\int_0^t\left[1-\frac{C(t)}{C(i)}\right]dt = [\,(18.6232-0)*1\,]-0.0054$$

$$= 18.6178\ cm^3\ g^{-1}\ adsorbent$$

$$q_{breakthrough} = \frac{0.692 * 0.0010490914 * 18.6178}{98.1624}$$

$$= 0.0001377\ mol\ g^{-1}\ adsorbent$$

$$= 0.1377\ mmol\ g^{-1}\ adsorbent$$

for saturation point

$$\frac{v}{m_{adsorbent}}\int_0^t\left[1-\frac{C(t)}{C(i)}\right]dt = [\,(342.1797-0)*1\,]-153.4078$$

$$= 188.7719\ cm^3\ g^{-1}\ adsorbent$$

$$q_{breakthrough} = \frac{0.692 * 0.0010490914 * 188.7719}{98.1624}$$

$= 0.001396$ mol g^{-1} adsorbent

$= 1.396$ mmol g^{-1} adsorbent

A2.2 Calculation the Percentage of Adsorption Capacity Recovery After Regeneration

Saturation capacity : Fresh NaX $= 1.3961$ mmol g^{-1} adsorbent

Regenerated NaX $= 1.2760$ mmol g^{-1} adsorbent

$$\% \text{ adsorption capacity recovery} = \frac{1.2760 * 100}{1.3961}$$

$$= 91.3978\ \%$$

Appendix B Experimenta! Data

Table B1 Breakthrough curve of 200 ppmw of 3-Methylthiophene in Isooctane on NaX zeolite

Time (min)	Concentration (ppmw)	Treated Volume (cm^3 g^{-1} adsorbent)	c(t)/c(i)
0	0.0000	0.0000	0.0000
1.5	0.0000	1.4828	0.0000
31.5	0.0000	31.1388	0.0000
41.5	7.6605	41.0241	0.0355
51.5	11.2601	50.9095	0.0522
61.5	21.2462	60.7948	0.0984
81.5	24.3328	80.5654	0.1127
101.5	30.1835	100.3361	0.1398
121.5	35.8041	120.1068	0.1659
151.5	47.7000	149.7628	0.2210
181.5	59.0569	179.4187	0.2736
201.5	65.6207	199.1894	0.3040
221.5	76.7642	218.9601	0.3556
241.5	83.3457	238.7307	0.3861
301.5	105.3723	298.0427	0.4882
361.5	117.0795	357.3547	0.5424
401.5	135.3743	396.8960	0.6272
421.5	138.6990	416.6667	0.6426
451.5	149.6264	446.3227	0.6932
481.5	157.7689	475.9786	0.7309
541.5	171.5799	535.2906	0.7949
601.5	183.0373	594.6026	0.8480
631.5	187.8653	624.2586	0.8703
661.5	192.8488	653.9146	0.8934
691.5	200.5829	683.5706	0.9293
721.5	200.2256	713.2266	0.9276
751.5	206.8289	742.8826	0.9582
811.5	214.3121	802.1945	0.9929

Note: Volumetric flow rate = 0.5 cm^3 min^{-1}

Total bed weight = 0.5058 g

Initial 3-methylthiophene concentration = 215.8538 ppmw

Table B2 Breakthrough curve of 500 ppmw of 3-Methylthiophene in Isooctane on NaX zeolite

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
1.5	0.0000	1.4837	0.0000
33.0	0.0000	32.6409	0.0000
42.5	10.4505	42.0376	0.0198
65.5	23.5417	64.7873	0.0447
82.5	34.0249	81.6024	0.0645
96.0	46.0496	94.9555	0.0874
113.0	68.7689	111.7705	0.1305
141.5	107.3758	139.9604	0.2037
183.5	161.1621	181.5035	0.3057
221.5	206.1343	219.0900	0.3911
241.5	254.3516	238.8724	0.4825
273.5	299.1464	270.5242	0.5675
301.5	344.4636	298.2196	0.6535
333.5	374.8947	329.8714	0.7112
361.5	402.0550	357.5668	0.7627
433.5	472.9500	428.7834	0.8972
452.5	482.7180	447.5767	0.9158
483.5	482.4255	478.2394	0.9152
515.5	514.6554	509.8912	0.9763
541.5	522.5893	535.6083	0.9914
571.5	533.2595	565.2819	1.0116
635.5	538.4129	628.5856	1.0214
721.5	540.8504	713.6499	1.0260

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5055 g

Initial 3-methylthiophene concentration = 527.1270 ppmw

Table B3 Breakthrough curve of 1000 ppmw of 3-Methylthiophene in Isooctane on fresh NaX zeolite (1 hrs for regeneration)

Time (min)	Concentration (ppmw)	Treated Volume (cm^3 g^{-1} adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
1.5	0.0000	1.4884	0.0000
6.5	0.0000	6.4497	0.0000
12.0	14.6081	11.9071	0.0135
31.5	24.5700	31.2562	0.0227
42.0	45.9948	41.6749	0.0424
53.0	77.1228	52.5898	0.0711
61.5	113.8122	61.0240	0.1049
81.5	201.1220	80.8692	0.1854
101.5	240.2481	100.7144	0.2215
121.5	293.9445	120.5596	0.2710
141.5	395.5978	140.4048	0.3647
161.5	492.3699	160.2500	0.4539
181.5	557.1835	180.0953	0.5137
201.5	692.3307	199.9405	0.6383
221.5	781.0540	219.7857	0.7200
241.5	837.9358	239.6309	0.7725
261.5	929.9327	259.4761	0.8573
281.5	946.1864	279.3213	0.8723
301.5	1028.1573	299.1665	0.9478
331.5	1061.9678	328.9343	0.9790
361.5	1059.7319	358.7021	0.9770
391.5	1093.7013	388.4699	1.0083
421.5	1113.8359	418.2377	1.0268

Note: Volumetric flow rate = 0.5 cm^3 min^{-1}

Total bed weight = 0.5039 g

Initial 3-methylthiophene concentration = 1084.7263 ppmw

Table B4 Breakthrough curve of 1000 ppmw of 3-Methylthiophene in Isooctane on regenerated NaX zeolite (1 hrs for regeneration)

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
2.5	21.4700	2.4807	0.0198
11.5	26.5875	11.4110	0.0245
21.5	35.6055	21.3336	0.0328
32.5	56.2346	32.2485	0.0518
41.5	79.2579	41.1788	0.0731
51.5	115.5600	51.1014	0.1065
61.5	150.2948	61.0240	0.1386
81.5	184.9262	80.8692	0.1705
101.5	268.4964	100.7144	0.2475
121.5	355.1547	120.5596	0.3274
141.5	451.2488	140.4048	0.4160
161.5	550.7939	160.2500	0.5078
181.5	651.0281	180.0953	0.6002
201.5	752.0925	199.9405	0.6933
221.5	822.2935	219.7857	0.7581
241.5	887.8086	239.6309	0.8185
261.5	986.0776	259.4761	0.9091
281.5	1044.4225	279.3213	0.9628
301.5	1065.1561	299.1665	0.9820
331.5	1089.4658	328.9343	1.0044
361.5	1055.0063	358.7021	0.9726
391.5	1109.8184	388.4699	1.0231

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5039 g

Initial 3-methylthiophene concentration = 1084.7263 ppmw

Table B5 Breakthrough curve of 1000 ppmw of 3-Methylthiophene in Isooctane on fresh NaX zeolite (3 hrs for regeneration)

Time (min)	Concentration (ppmw)	Treated Volume (cm^3 g^{-1} adsorbent)	c(t)/c(i)
0	0.0000	0.0000	0.0000
2.5	0.0000	2.4802	0.0000
11.5	0.0000	11.4087	0.0000
16.5	0.0000	16.3690	0.0000
21.5	11.0028	21.3294	0.0105
26.5	27.4856	26.2897	0.0262
31.5	20.6876	31.2500	0.0197
36.5	30.9370	36.2103	0.0295
41.5	32.9136	41.1706	0.0314
52.0	48.4551	51.5873	0.0462
61.5	66.9748	61.0119	0.0638
81.5	116.0978	80.8532	0.1107
101.5	118.3906	100.6944	0.1129
121.5	245.5185	120.5357	0.2340
141.5	297.7734	140.3770	0.2838
161.5	399.3960	160.2183	0.3807
181.5	476.0756	180.0595	0.4538
201.5	582.0710	199.9008	0.5548
221.5	661.2140	219.7421	0.6303
241.5	765.5520	239.5833	0.7297
261.5	826.6035	259.4246	0.7879
281.5	900.1947	279.2659	0.8581
301.5	966.0306	299.1071	0.9208
331.5	987.3407	328.8690	0.9411
361.5	1008.1556	358.6310	0.9610
391.5	1029.85508	388.3929	0.9817
421.5	1071.6793	418.1548	1.0215

Note: Volumetric flow rate = 0.5 cm^3 min^{-1}

Total bed weight = 0.5040 g

Initial 3-methylthiophene concentration = 1049.0914 ppmw

Table B6 Breakthrough curve of 1000 ppmw of 3-Methylthiophene in Isooctane on regenerated NaX zeolite (3 hrs for regeneration)

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0	0.0000	0.0000	0.0000
2.5	33.8526	2.4802	0.0323
11.5	11.8875	11.4087	0.0113
16.5	0.0000	16.3690	0.0000
26.5	14.0239	26.2897	0.0134
31.5	20.6102	31.2500	0.0196
36.5	20.6102	36.2103	0.0196
41.5	39.5190	41.1706	0.0377
46.5	52.0698	46.1310	0.0496
56.5	72.4065	56.0516	0.0690
71.5	95.9796	70.9325	0.0915
81.5	137.8437	80.8532	0.1314
101.5	200.3225	100.6944	0.1909
121.5	287.2977	120.5357	0.2739
141.5	362.3172	140.3770	0.3454
161.5	466.6222	160.2183	0.4448
181.5	577.0890	180.0595	0.5501
201.5	687.5013	199.9008	0.6553
221.5	726.2607	219.7421	0.6923
241.5	854.3924	239.5833	0.8144
261.5	925.0146	259.4246	0.8817
281.5	918.0977	279.2659	0.8751
301.5	1019.4068	299.1071	0.9717
343.5	1049.5915	340.7738	1.0005
391.5	1043.1718	388.3929	0.9944
421.5	1041.5255	418.1548	0.9928

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5040 g

Initial 3-methylthiophene concentration = 1060.5815 ppmw

Table B7 Breakthrough curve of 1800 ppmw of 3-Methylthiophene in Isooctane on NaX zeolite

Time (min)	Concentration (ppmw)	Treated Volume (cm^3 g^{-1} adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
1.5	29.7491	1.4872	0.0153
6.5	36.1749	6.4446	0.0186
16.5	94.6448	16.3593	0.0488
26.5	156.9786	26.2740	0.0809
31.5	191.8091	31.2314	0.0988
41.5	262.1908	41.1461	0.1351
51.5	353.8619	51.0609	0.1824
62.5	468.5828	61.9671	0.2415
81.5	709.5481	80.8051	0.3656
101.5	1018.3193	100.6345	0.5248
121.5	1283.7053	120.4640	0.6615
141.5	1554.8456	140.2935	0.8012
161.5	1705.5733	160.1229	0.8789
181.5	1866.9800	179.9524	0.9621
201.5	1902.1547	199.7819	0.9802
221.5	1988.6438	219.6113	1.0248
241.5	1950.5148	239.4408	1.0051
281.5	1965.8093	279.0997	1.0130

Note: Volumetric flow rate = 0.5 cm^3 min^{-1}

Total bed weight = 0.5043 g

Initial 3-methylthiophene concentration = 1940.5416 ppmw

Table B8 Breakthrough curve of 200 ppmw of Benzothiophene in Isooctane on NaX zeolite

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
41.5	0.0000	41.0485	0.0000
61.5	5.9741	60.8309	0.0257
84.5	8.1277	83.5806	0.0350
101.5	10.3621	100.3956	0.0447
121.5	12.3071	120.1780	0.0530
151.5	15.7250	149.8516	0.0678
181.5	20.0303	179.5252	0.0863
241.5	33.9799	238.8724	0.1464
301.5	44.1097	298.2196	0.1901
361.5	58.8590	357.5668	0.2536
421.5	69.6355	416.9139	0.3001
481.5	90.3716	476.2611	0.3894
541.5	98.2664	535.6083	0.4234
601.5	112.7284	594.9555	0.4858
661.5	130.8168	654.3027	0.5637
721.5	143.9609	713.6499	0.6204
781.5	159.6488	772.9970	0.6880
841.5	179.2597	832.3442	0.7725
901.5	185.7447	891.6914	0.8004
961.5	190.3665	951.0386	0.8203
1081.5	218.3513	1069.7329	0.9409
1201.5	229.4032	1188.4273	0.9885
1321.5	233.4416	1307.1217	1.0059
1381.5	233.2541	1366.4688	1.0051

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5055 g

Initial benzothiophene concentration = 232.0635 ppmw

Table B9 Breakthrough curve of 500 ppmw of Benzothiophene in Isooctane on NaX zeolite

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
5.0	0.0000	4.9456	0.0000
61.5	0.0000	60.8309	0.0000
71.5	6.0564	70.7221	0.0125
84.5	16.0497	83.5806	0.0332
141.5	35.0852	139.9604	0.0725
181.5	61.2076	179.5252	0.1265
241.5	111.5650	238.8724	0.2305
303.5	141.1118	300.1978	0.2916
331.5	168.9867	327.8932	0.3492
361.5	207.5901	357.5668	0.4290
421.5	266.9112	416.9139	0.5516
483.5	307.8538	478.2394	0.6362
541.5	400.9941	535.6083	0.8286
609.0	433.1636	602.3739	0.8951
691.5	502.0772	683.9763	1.0375
723.5	498.0030	715.6281	1.0291
794.5	492.0919	785.8556	1.0169
904.6	512.0656	894.7577	1.0581

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5055 g

Initial benzothiophene concentration = 483.9290 ppmw

Table B10 Breakthrough curve of 1000 ppmw of Benzothiophene in Isooctane on fresh NaX zeolite (1 hrs for regeneration)

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
1.5	0.0000	1.4878	0.0000
11.5	0.0000	11.4065	0.0000
21.5	0.0000	21.3251	0.0000
26.5	0.0000	26.2845	0.0000
31.5	11.3752	31.2438	0.0102
41.5	19.8903	41.1625	0.0178
51.5	33.4267	51.0811	0.0298
61.5	48.2574	60.9998	0.0431
81.5	58.7309	80.8371	0.0524
101.5	78.4486	100.6745	0.0700
121.5	136.8200	120.5118	0.1221
141.5	265.9136	140.3491	0.2374
151.5	313.4294	150.2678	0.2798
161.5	376.4194	160.1865	0.3360
181.5	427.3992	180.0238	0.3815
201.5	532.3606	199.8611	0.4752
241.5	724.1097	239.5358	0.6464
261.5	830.5395	259.3731	0.7414
281.5	866.8252	279.2105	0.7738
301.5	941.7828	299.0478	0.8407
331.5	1031.9602	328.8038	0.9212
361.5	1094.0694	358.5598	0.9766
391.5	1114.6832	388.3158	0.9950
421.5	1144.6185	418.0718	1.0217
452.0	1127.3739	448.3237	1.0063
481.5	1131.9628	477.5838	1.0104
511.5	1147.6886	507.3398	1.0245

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5041 g

Initial benzothiophene concentration = 1120.2707 ppmw

Table B11 Breakthrough curve of 1000 ppmw of Benzothiophene in Isooctane on regenerated NaX zeolite (1 hrs for regeneration)

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
1.5	11.4405	1.4878	0.0102
21.5	7.9861	21.3251	0.0071
32.5	12.4392	32.2357	0.0111
41.5	13.2065	41.1625	0.0118
51.5	34.9242	51.0811	0.0312
61.5	34.9242	60.9998	0.0312
81.5	70.1163	80.8371	0.0626
112.5	143.5764	111.5850	0.1282
122.5	259.1290	121.5037	0.2313
141.5	343.2607	140.3491	0.3064
161.5	487.5358	160.1865	0.4352
181.5	580.3777	180.0238	0.5181
201.5	637.8118	199.8611	0.5693
222.5	842.4228	220.6903	0.7520
242.5	839.9519	240.5277	0.7498
261.5	954.1280	259.3731	0.8517
281.5	1002.0102	279.2105	0.8944
304.5	1040.4104	302.0234	0.9287
321.5	1088.2082	318.8851	0.9714
361.5	1107.2777	358.5598	0.9884
381.5	1149.6272	378.3971	1.0262
421.5	1142.5942	418.0718	1.0199
441.5	1138.0220	437.9091	1.0158

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5041 g

Initial benzothiophene concentration = 1120.2707 ppmw

Table B12 Breakthrough curve of 1000 ppmw of Benzothiophene in Isooctane on fresh NaX zeolite (3 hrs for regeneration)

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
1.5	0.0000	1.4878	0.0000
11.5	0.0000	11.4065	0.0000
21.5	0.0000	21.3251	0.0000
31.5	0.0000	31.2438	0.0000
53.0	6.4668	52.5689	0.0059
62.5	13.5301	61.9917	0.0124
81.5	28.9194	80.8371	0.0266
101.5	49.1691	100.6745	0.0452
121.5	90.3472	120.5118	0.0830
141.5	151.9301	140.3491	0.1396
161.5	232.8836	160.1865	0.2141
181.5	334.6991	180.0238	0.3076
203.5	448.5325	201.8449	0.4123
222.5	546.3279	220.6903	0.5022
261.5	745.9153	259.3731	0.6856
287.0	833.8252	284.6657	0.7664
302.5	886.6882	300.0397	0.8150
331.5	966.8274	328.8038	0.8887
362.5	1027.6699	359.5517	0.9446
391.5	1042.8873	388.3158	0.9586
421.5	1109.9921	418.0718	1.0203
452.0	1107.5770	448.3237	1.0180
481.5	1102.5087	477.5838	1.0134
541.5	1097.3936	537.0958	1.0087
601.5	1100.2445	596.6078	1.0113

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5040 g

Initial benzothiophene concentration = 1087.9565 ppmw

Table B13 Breakthrough curve of 1000 ppmw of Benzothiophene in Isooctane on regenerated NaX zeolite (3 hrs for regeneration)

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
1.5	5.9665	1.4878	0.0055
11.5	13.0053	11.4065	0.0120
36.5	17.4796	36.2031	0.0161
45.5	20.2533	45.1299	0.0186
52.5	22.2914	52.0730	0.0205
61.5	38.9193	60.9998	0.0358
85.5	61.3826	84.8046	0.0564
101.5	129.8873	100.6745	0.1194
131.5	193.5733	130.4305	0.1779
153.0	304.5265	151.7556	0.2799
173.5	446.6412	172.0889	0.4105
201.5	577.6086	199.8611	0.5309
225.5	683.6667	223.6659	0.6284
242.5	693.6076	240.5277	0.6375
272.5	829.4130	270.2837	0.7624
301.5	933.4726	299.0478	0.8580
331.5	1050.0182	328.8038	0.9651
362.5	1048.0052	359.5517	0.9633
391.5	1090.0589	388.3158	1.0019
421.5	1103.6498	418.0718	1.0144
451.5	1111.2145	447.8278	1.0214
481.5	1113.4516	477.5838	1.0234

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5040 g

Initial benzothiophene concentration = 1087.9565 ppmw

Table B14 Breakthrough curve of 1800 ppmw of Benzothiophene in Isooctane on NaX zeolite.

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
1.5	19.4708	1.4749	0.0112
6.5	16.0504	6.3913	0.0092
12.0	12.8292	11.7994	0.0074
16.5	10.4161	16.2242	0.0060
21.5	13.6474	21.1406	0.0079
26.5	23.4469	26.0570	0.0135
31.5	35.6559	30.9735	0.0205
36.5	52.1985	35.8899	0.0301
41.5	84.0155	40.8063	0.0484
47.5	130.6695	46.7060	0.0752
56.5	206.4517	55.5556	0.1189
61.5	292.0206	60.4720	0.1681
71.5	336.8379	70.3048	0.1939
81.5	460.1854	80.1377	0.2649
91.5	602.2530	89.9705	0.3467
121.5	899.4718	119.4690	0.5178
151.5	1176.3134	148.9676	0.6772
187.0	1593.7012	183.8741	0.9175
210.5	1714.1180	206.9813	0.9868
242.5	1769.5944	238.4464	1.0188
271.5	1764.6342	266.9617	1.0159
331.5	1752.8246	325.9587	1.0091

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5085 g

Initial benzothiophene concentration = 1736.9782 ppmw

Table B15 Breakthrough curve of 200 ppmw of Dibenzothiophene in Decane on NaX zeolite

Time (min)	Concentration (ppmw)	Treated Volume (cm^3 g^{-1} adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
21.5	0.0000	21.3845	0.0000
41.5	10.9776	41.2771	0.0485
61.5	18.8261	61.1697	0.0832
81.5	27.3369	81.0623	0.1209
101.5	31.5897	100.9548	0.1397
121.5	37.3740	120.8474	0.1652
141.5	41.4318	140.7400	0.1832
161.5	45.2107	160.6326	0.1999
181.5	52.4450	180.5252	0.2319
211.5	64.2289	210.3640	0.2840
271.5	80.9698	270.0418	0.3580
331.5	92.1159	329.7195	0.4073
391.5	103.8464	389.3973	0.4591
451.5	119.3291	449.0750	0.5276
511.5	127.9441	508.7527	0.5657
571.5	133.7232	568.4305	0.5912
631.5	146.6488	628.1082	0.6484
661.5	150.7501	657.9471	0.6665
721.5	155.6702	717.6248	0.6883
751.5	163.5165	747.4637	0.7230
841.5	170.3406	836.9803	0.7531
901.5	176.4548	896.6580	0.7802
961.5	182.1052	956.3358	0.8052
1021.5	193.5381	1016.0135	0.8557
1081.5	201.4440	1075.6913	0.8907
1141.5	208.9009	1135.3690	0.9236
1201.5	213.6427	1195.0467	0.9446
1261.5	220.7727	1254.7245	0.9761

Note: Volumetric flow rate = 0.5 cm^3 min^{-1}

Total bed weight = 0.5027 g

Initial dibenzothiophene concentration = 226.1731 ppmw

Table B16 Breakthrough curve of 500 ppmw of Dibenzothiophene in Decane on NaX zeolite

Time (min)	Concentration (ppmw)	Treated Volume (cm^3 g^{-1} adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
22.5	0.0000	22.2993	0.0000
41.5	17.7036	41.1298	0.0338
61.5	49.4159	60.9514	0.0944
81.5	67.7039	80.7730	0.1293
103.0	95.4751	102.0813	0.1823
122.5	122.2409	121.4073	0.2334
141.5	141.7662	140.2379	0.2707
161.5	162.1664	160.0595	0.3097
182.5	180.4679	180.8722	0.3446
217.5	210.7861	215.5600	0.4025
276.5	253.4677	274.0337	0.4841
337.0	286.8608	333.9941	0.5478
391.5	347.0972	388.0079	0.6629
451.5	387.5385	447.4727	0.7401
511.5	434.5278	506.9376	0.8298
571.5	463.0152	566.4024	0.8842
631.5	476.7085	625.8672	0.9104
721.5	501.5686	715.0644	0.9579
781.5	518.4544	774.5292	0.9901
841.5	543.857066	833.9941	1.0386
961.5	534.6928	952.9237	1.0211

Note: Volumetric flow rate = 0.5 cm^3 min^{-1}

Total bed weight = 0.5045 g

Initial dibenzothiophene concentration = 523.6335 ppmw

Table B17 Breakthrough curve of 1000 ppmw of Dibenzothiophene in Decane on fresh NaX zeolite (3 hrs for regeneration)

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
1.5	0.0000	1.4890	0.0000
11.5	6.2394	11.4155	0.0056
21.5	20.7214	21.3421	0.0186
31.5	43.1980	31.2686	0.0389
41.5	65.5790	41.1952	0.0590
53.5	100.1105	53.1070	0.0901
62.5	119.6943	62.0409	0.1077
82.5	178.6893	81.8940	0.1608
101.5	244.2139	100.7544	0.2198
123.5	323.5470	122.5928	0.2912
142.5	406.5710	141.4532	0.3659
161.5	476.4842	160.3137	0.4288
181.5	568.9958	180.1668	0.5121
204.5	649.4067	202.9978	0.5844
221.5	711.4357	219.8729	0.6402
241.5	786.2685	239.7260	0.7076
271.5	863.9507	269.5057	0.7775
301.5	923.9128	299.2853	0.8315
331.5	996.8846	329.0649	0.8971
361.5	1036.4854	358.8446	0.9328
391.5	1072.1082	388.6242	0.9648
421.5	1110.6346	418.4038	0.9995
451.5	1158.4394	448.1834	1.0425

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5037 g

Initial dibenzothiophene concentration = 1111.1918 ppmw

Table B18 Breakthrough curve of 1000 ppmw of Dibenzothiophene in Decane on regenerated NaX zeolite (3 hrs for regeneration)

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0	0.0000	0.0000	0.0000
1.5	510.4830	1.4890	0.4594
13.5	603.2707	13.4008	0.5429
26.5	625.9793	26.3053	0.5633
36.5	677.6431	36.2319	0.6098
46.5	685.0389	46.1584	0.6165
71.5	730.6554	70.9748	0.6575
91.5	774.0009	90.8279	0.6966
113.5	870.9040	112.6663	0.7838
131.5	950.7780	130.5340	0.8556
151.5	992.5050	150.3871	0.8932
171.5	1033.0767	170.2402	0.9297
201.5	1033.0767	200.0199	0.9297
221.5	1079.5383	219.8729	0.9715
241.4	1091.9476	239.6268	0.9827
271.5	1114.6830	269.5057	1.0031

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5037 g

Initial dibenzothiophene concentration = 1111.1918 ppmw

Table B19 Breakthrough curve of 1800 ppmw of Dibenzothiophene in Decane on NaX zeolite

Time (min)	Concentration (ppmw)	Treated Volume ($cm^3\ g^{-1}$ adsorbent)	c(t)/c(i)
0.0	0.0000	0.0000	0.0000
1.5	0.0000	1.4890	0.0000
6.5	9.2883	6.4523	0.0049
11.5	14.8545	11.4155	0.0079
21.5	125.7457	21.3421	0.0668
31.5	245.4613	31.2686	0.1303
43.0	402.2007	42.6841	0.2136
52.0	492.6366	51.6180	0.2616
61.5	631.0267	61.0482	0.3351
81.5	840.6776	80.9013	0.4464
101.5	1026.2017	100.7544	0.5449
121.5	1261.2556	120.6075	0.6697
141.5	1350.9761	140.4606	0.7173
161.5	1407.9414	160.3137	0.7476
181.5	1637.2806	180.1668	0.8693
201.5	1773.3528	200.0199	0.9416
221.5	1809.1725	219.8729	0.9606
241.5	1861.9516	239.7260	0.9886
261.5	1898.3273	259.5791	1.0079
281.5	1908.7527	279.4322	1.0135
301.5	1879.7902	299.2853	0.9981

Note: Volumetric flow rate = 0.5 $cm^3\ min^{-1}$

Total bed weight = 0.5037 g

Initial dibenzothiophene concentration = 1883.3568 ppmw

Appendix C Bed Voidage

The fractional void in the packed column could be obtained from Figure A1.

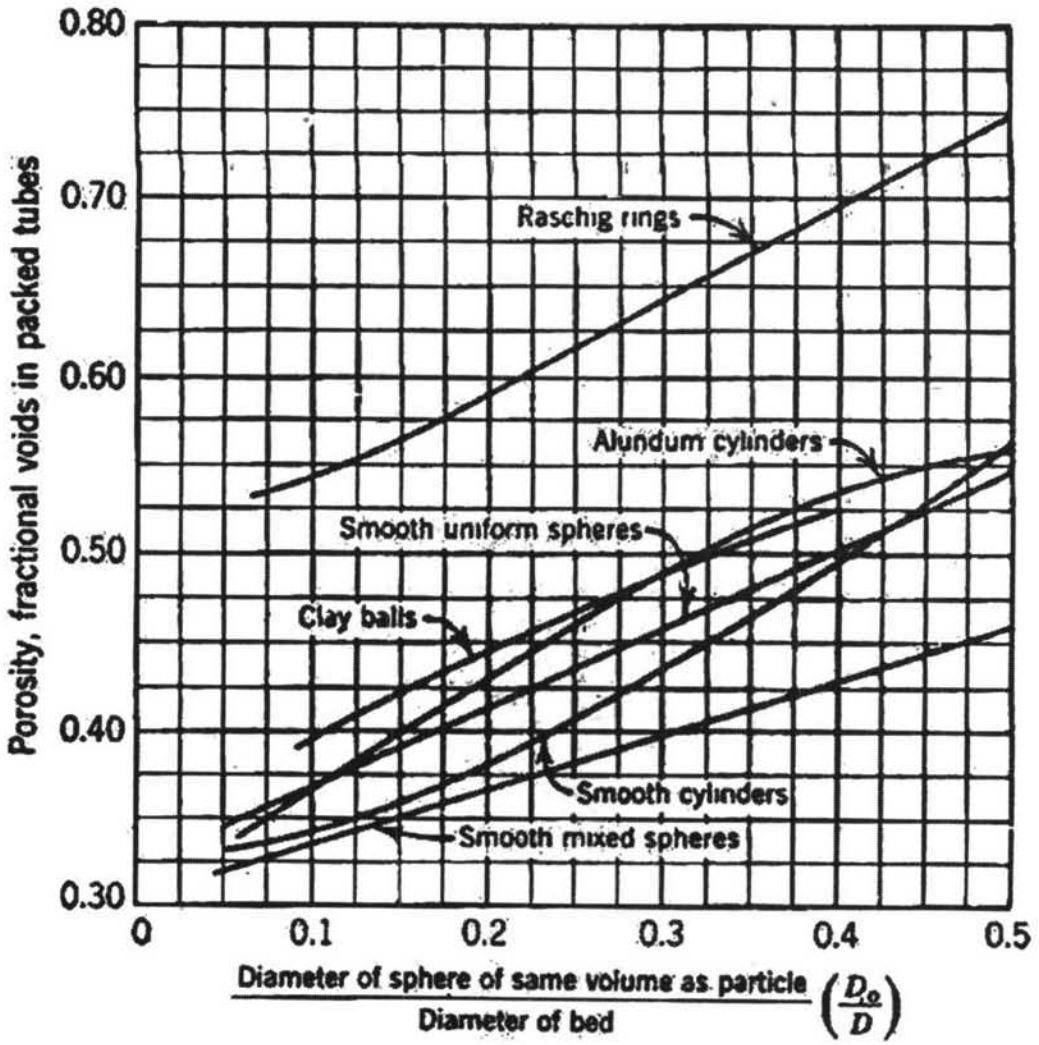

Figure C1 Porosity as a function of the ratio of particle diameter to bed diameter. (Leva, 1974)

Appendix D Correlations Relating to the Model

D.1 Axial Dispersion Coefficient

The axial dispersion coefficient (D_L) which was lumped parameter accounted for the effects of all mechanisms with contribute to axial mixing was calculated by (Koch and Brandy, 1985).

$$\frac{D_L A}{Q d_p} = \varepsilon_b \left[\frac{3}{4} + \frac{\pi^2}{6}(1-\varepsilon_b)\ln(Pe_{Mp}) + \frac{1}{Pe_{Mp}} \right] \tag{D1.1}$$

Where Q is volumetric flow rate. A is cross section area of column and ε_b is bed porosity. The molecular mass Peclet number for the particle defined by

$$Pe_{Mp} = \frac{v_z d_p \varepsilon_b}{D_{AB}} \tag{D1.2}$$

The diffusion coefficient estimated by Wilke and Chang equation (1995), for dilute system

$$\frac{D_{AB}\mu_B}{T} = 7.4 \times 10^{-8} \frac{(\phi M_B)^{0.5}}{V_{b_A}^{0.6}} \tag{D1.3}$$

Where ø (association parameter) = 1 for hydrocarbon, V_{bA} the molar volume of solute (cm^3 mole-1). μ_B the viscosity of solvent (centipoises), T temperature (K) and M_B is molecular weight of solvent (g $mole^{-1}$).

D.2 Mass Transfer Coefficient

The mass transfer coefficient K_m in the fixed bed is calculated using the following correlation for Sherwood number defined as the following

$$Sh = \frac{2K_m R_p}{D_m} \tag{D2.1}$$

$$Sh = 2.0 + 1.1(Sc)^{0.33}(\mathrm{Re})^{0.6} \tag{D2.2}$$

D.3 Effective Diffusivity in the Pores

The effective diffusivity inside the pores is determined using the formula:

$$D_P = \frac{D\varepsilon_P}{\tau} \tag{D3.1}$$

The combined diffusivity, D inside the macro-pores of the zeolite pellet is given by a combination of both Knudsen (D_k) and molecular (D_{AB}) diffusivities as:

$$\frac{1}{D} = \frac{1}{D_k} + \frac{1}{D_{AB}} \tag{D3.2}$$

Where, Knudsen diffusivity is given as, D_k (m^2/s) = $97R_{pore}[T(^oC)/ MW_{sulfur}]^{1/2}$.

Appendix E Simulation Program for MATLAB™ Model

This program was developed for solving the sets of the mass and adsorption equation in order to construct the theoretical breakthrough curves. The method of lines (MOLs) with central finite difference approximatation and ODE45 solver provided by MATLAB™ program were employed to solve the partial differential equations.

```
function Conc
=Breakthrough5(t,c,options,h,V,voidb,voidp,a,DL,Cin,Nsegment,Km,Dp,Rp)
a
Conc = zeros(2*Nsegment,1);

X =( Km/((Km+5*Dp/Rp)*voidp))*a;
Y = (15*(1-voidb)*Km*Dp)/(voidb*Rp^2*(Km+5*Dp/Rp));

% First section %
Conc(1) = (DL/(h^2*voidb))*(c(2)-2*c(1)+Cin)-(V/(2*h*voidb))*(c(2)-Cin)-Y*(c(1)-
c(Nsegment+1));
Conc(Nsegment+1) = -(c(1)-c(Nsegment+1))*X;

% Section 2-(Nsegmet-1) %
for i = 2:1:(Nsegment-1)
Conc(i) = (DL/(h^2*voidb))*(c(i+1)-2*c(i)+c(i-1))-(V/(2*h*voidb))*(c(i+1)-c(i-1))-
Y*(c(i)-c(Nsegment+i));
Conc(Nsegment+i) = -(c(i)-c(Nsegment+i))*X;
end;

% Last section %
Conc(Nsegment) = (DL/(h^2*voidb))*(2*c(Nsegment-1)-2*c(Nsegment))-
Y*(c(Nsegment)-c(2*Nsegment));
Conc(2*Nsegment) = -(c(Nsegment)-c(2*Nsegment))*X;
```

```
clear all;
Nsegment = 50;
h = 0.05/Nsegment;
V = 5.0413E-04;                 % m/s
voidb = 0.325;
voidp = 0.3;
a = [-5E-05];
Km = 1.43478E-05;               % m/s
Dp = 2.94133E-10;               % m2/s
Rp = 0.000320812;               % m  (pellet diameter)
DL = 5.82E-07;                  % m2/s
Cin = 1.9945163;                % mol/m3  (1800 ppmW S)
Settime = 100:100:80000;
L = 0.05                        % Adsorber length
Conc = zeros(size(a,2),(Nsegment+1));
for m = 1:length(Settime)
time = 0:100:Settime(m);
l= 0:(L/Nsegment):L;
NumPDE = 2*Nsegment;
for i = 1:size(a,2);
[t,y] = ode45
('Breakthrough5',time,[zeros(NumPDE,1)],[],h,V,voidb,voidp,a,DL,Cin,Nsegment,Km,
Dp,Rp);
Cin1 = Cin*ones(size(t,1),1);
Y1 = [Cin1,y];
Conc(i,:) = Y1(size(t,1),1:(Nsegment+1));
end;
Cexit(m) = Conc(i,(Nsegment+1));
end;
Cratio = Cexit/Cin;
plot(Settime/60, Cratio,'g');
      title('Breakthrogh Curve')
      xlabel('fuel vol (cm3/g cat)')
      ylabel('C(t)/C(i)')
```

Appendix F Simulation parameters

Table F1 The physical properties and simulation parameters

Parameter	Unit	3-MT	BT	DBT
Pellet voidage, ε_P	-	0.3	0.3	0.3
Bed voidage, ε_b	-	0.325	0.325	0.325
Average mass transfer coefficient, K_m	m s^{-1}	2.90E-05	2.64E-05	1.43E-05
Pellet radius, R_p	m	3.21E-04	3.21E-04	3.21E-04
Interstitial fluid velocity, v_z	m s^{-1}	5.04E-04	5.04E-04	5.04E-04
Axial dispersion coefficient, D_L	m^2 s^{-1}	4.93E-07	5.06E-07	5.82E-07
Knudsen diffusivity, D_k	m^2 s^{-1}	3.62E-08	3.10E-08	2.64E-08
molecular diffusivity, D_{AB}	cm^2 s^{-1}	3.03E-05	2.69E-05	1.39E-05
Combined diffusivity inside the macro-pores of the zeolites pellet, D	m^2 s^{-1}	2.80E-09	2.48E-09	1.32E-09
Effective diffusivity inside the pores, D_p	m^2 s^{-1}	6.22E-10	5.51E-10	2.94E-10
Density of solvent, ρ	g cm^{-3}	0.692	0.692	0.735
Density of sulfur compound, ρ_s	g cm^{-3}	1.016	1.14	1.20
Viscosity of solvent, μ	poise	0.005	0.005	0.0092
Molecular weight of sulfur compound, Mw	g mol^{-1}	96.585	117.715	153.546
Molar volume of sulfur compound, V_{bA}	cm^3 mol^{-1}	96.585	117.715	153.546
Diameter of bed, d_b	cm	0.44	0.44	0.44

Parameters	Unit	3-MT	BT	DBT
Temperature, T	°C	25	25	25
Tortuosity factor, τ	-	1.35	1.35	1.35
Schmidt number, *Sc*	-	238.16	268.18	898.34
Reynold number, *Re*	-	0.4477	0.4477	0.2584
Concentration 200 ppmw	mol m^{-3}	1.4099	1.0313	0.7978
Concentration 500 ppmw	mol m^{-3}	3.5248	2.5783	1.9945
Concentration 1000 ppmw	mol m^{-3}	7.0495	5.1567	3.9890
Concentration 1800 ppmw	mol m^{-3}	12.6892	9.2820	7.1803

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