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APPENDICES

APPENDIX A Calculation and Samples of Calculation

A1 Calculations of Amount of Metal Loading on NaX and NaY Zeolite

A1.1 Amount of Metal Loading on Zeolite

From

$$\begin{aligned}C_{i2} &= C_{i1} * T \\M &= C_{i2} * V_0 * 10^{-6} \\ \%Wt &= \frac{M}{A_0} * 100\end{aligned}\quad (A1.1.1)$$

Where,

- C_{i2} = Concentration before dilution ($\mu\text{g/ml}$)
- C_{i1} = Concentration after dilution of metal solution ($\mu\text{g/ml}$)
- T = Times of dilution
- M = Amount of metal loading on zeolite (g)
- V_0 = Initial volume of metal solution (ml)
- $\%Wt$ = Weight percent (%)
- A_0 = Weight of initial adsorbent (g)

Example: Amount of Ni^{2+} loading on NaX zeolite at room temperature (solution : adsorbent = 200)

$$\begin{aligned}\text{Result data from AAS } (C_{Ni1}) &= 3.297 \mu\text{g/ml} \\ \text{Times of dilution } (T) &= 25 \\ \text{Therefore, concentration before dilution } (C_{Ni2}) &= 3.297 * 25 \\ &= 82.43 \mu\text{g/ml} \\ \\ \text{Initial volume of metal solution } (V_0) &= 100 \text{ ml} \\ \text{So, amount of metal loading on NaY zeolite} &= 82.43 * 100 * 10^{-6} \\ &= 0.008243 \text{ g} \\ \text{Weight of initial adsorbent } (A_0) &= 0.1208 \text{ g}\end{aligned}$$

$$\begin{aligned} \text{Weight percent (\%Wt)} &= \frac{0.008243}{0.1208} \times 100 \\ &= 6.82 \% \end{aligned}$$

A1.2 Ion-exchange isotherm by liquid phase ion-exchange technique

$$E_{A(S)} = \frac{z_A n_{A(S)}}{\sum_i z_i n_{i(S)}} \quad (\text{A1.1.2})$$

$$E_A = \frac{z_A n_A}{\sum_i z_i n_i} \quad (\text{A1.1.3})$$

Where,

$E_{A(S)}$ = Equivalent fraction of the cations present within the solution phase

E_A = Equivalent fraction of the cations present within the zeolite

z_A, z_i = Valencies of exchanging cations A and i

$n_{A(S)}, n_{i(S)}$ = Moles per unit volume of A and i within solution phase (mmol/ml)

n_A, n_i = Moles per unit volume of A and i within zeolite (mmol/ml)

Example: Amount of $E_{A(S)}$ of NaX zeolite (solution : adsorbent = 200)

In solution,

Ni^{2+} : Result data from AAS = 1.31 $\mu\text{g/ml}$

Times of dilution = 100

Therefore, concentration before dilution = 1.31 * 100
= 131 $\mu\text{g/ml}$

Moles per unit volume of Ni^{2+} within zeolite (n_{Ni}) = 0.00223 mmol/ml

Valencies of Ni^{2+} (z_{Ni}) = +2

Thus, $z_{\text{Ni}} * n_{\text{Ni}}$ = 0.00223 * 2

= 0.00446 mmol/ml

$$\begin{aligned}
 \text{Na}^+ : \text{ Result data from AAS } (n_{\text{Na}}) &= 0.092 \text{ } \mu\text{g/ml} \\
 \text{Times of dilution} &= 2500 \\
 \text{Therefore, concentration before dilution} &= 0.092 * 2500 \\
 &= 230 \text{ } \mu\text{g/ml} \\
 \text{Moles per unit volume of Na}^+ \text{ within zeolite } (n_{\text{Na}}) &= 0.00996 \text{ mmol/ml} \\
 \text{Valencies of Na}^{2+} (z_{\text{Na}}) &= +1 \\
 \text{Thus, } z_{\text{Na}} * n_{\text{Na}} &= 0.00996 * 1 \\
 &= 0.00996 \text{ mmol/ml}
 \end{aligned}$$

$$\text{So, } E_{\text{Ni(S)}} = \frac{0.00446}{0.00446 + 0.00996} = 0.31$$

In zeolite,

$$\begin{aligned}
 \text{Ni}^{2+} : \text{ Result data from AAS} &= 3.732 \text{ } \mu\text{g/ml} \\
 \text{Times of dilution} &= 25 \\
 \text{Therefore, concentration before dilution} &= 3.732 * 25 \\
 &= 93.31 \text{ } \mu\text{g/ml} \\
 \text{Moles per unit volume of Ni}^{2+} \text{ within zeolite } (n_{\text{Ni}}) &= 0.00159 \text{ mmol/ml} \\
 \text{Valencies of Ni}^{2+} (z_{\text{Ni}}) &= +2 \\
 \text{Thus, } z_{\text{Ni}} * n_{\text{Ni}} &= 0.00159 * 2 \\
 &= 0.00318 \text{ mmol/ml}
 \end{aligned}$$

$$\begin{aligned}
 \text{Na}^+ : \text{ Result data from AAS } (n_{\text{Na}}) &= 0.314 \text{ } \mu\text{g/ml} \\
 \text{Times of dilution} &= 100 \\
 \text{Therefore, concentration before dilution} &= 0.314 * 100 \\
 &= 314 \text{ } \mu\text{g/ml} \\
 \text{Moles per unit volume of Ni}^{2+} \text{ within zeolite } (n_{\text{Na}}) &= 0.00137 \text{ mmol/ml} \\
 \text{Valencies of Na}^{2+} (z_{\text{Na}}) &= +1 \\
 \text{Thus, } z_{\text{Na}} * n_{\text{Na}} &= 0.00137 * 1 \\
 &= 0.00137 \text{ mmol/ml}
 \end{aligned}$$

$$So, E_{Ni} = \frac{0.00318}{0.00318 + 0.00137} = 0.7$$

A1.3 Ion-exchange degree by solid state ion-exchange technique

$$\% \text{ Exchanged} = \frac{N_{Ni^{2+}} \times 2}{N_{Na^+} \times 1} * 100\% \quad (A1.1.4)$$

Where,

$N_{Ni^{2+}}$ = Moles of Ni^{2+} on zeolite after exchanged (g)

N_{Na^+} = Moles of Na^+ on zeolite before exchanged (g)

Example:

Ni^{2+} : Result data from AAS	= 4.759 $\mu\text{g/ml}$
Times of dilution	= 25
Therefore, concentration before dilution	= 4.759 * 25
	= 118.97 $\mu\text{g/ml}$
Initial volume of metal solution (V_o)	= 100 ml
So, amount of metal loading on NaY zeolite	= 118.97 * 100 * 10^{-6}
	= 0.011897 g
Weight of initial adsorbent (A_o)	= 0.1298 g
Moles of Ni^{2+} on zeolite after exchanged	= $\frac{0.011897}{0.1298 \times 58.71}$
	= 0.1561(mole/g-zeolite)

Na^+ : Result data from AAS	= 0.03287 $\mu\text{g/ml}$
Times of dilution	= 2500
Therefore, concentration before dilution	= 0.03287 * 2500
	= 82.18 $\mu\text{g/ml}$
Initial volume of metal solution (V_o)	= 100 ml
So, amount of metal loading on NaY zeolite	= 82.18 * 100 * 10^{-6}
	= 0.008218 g
Weight of initial adsorbent (A_o)	= 0.1145 g

$$\begin{aligned} \text{Moles of Na}^+ \text{ on zeolite before exchanged} &= \frac{0.008218}{0.1145 \times 23} \\ &= 0.31205(\text{mole/gzeolite}) \end{aligned}$$

$$\% \text{ Exchanged} = \frac{0.1561 \times 2}{0.31205 \times 1} * 100 \% = 100.06 \%$$

A2 Calculation of Sulfur Concentration (or Benzene) in static adsorption experiment

A2.1 Calibration of Sulfur Compounds (or Benzene)

From

$$\begin{aligned} n_i * \text{RMR}_i &= A_i \\ n_{\text{std}} * \text{RMR}_{\text{std}} &= A_{\text{std}} \end{aligned}$$

So,

$$\text{RMR}_i = \frac{A_i * n_{\text{std}} (\text{RMR}_{\text{std}})}{A_{\text{std}} * n_i} \quad (\text{A2.1.1})$$

A2.2 Concentration of Sulfur Compounds (or Benzene) in Simulated Fuels

$$Y_i = \frac{A_i / \text{RMR}_i}{\sum_{i=1}^n [A_i / \text{RMR}_i]} \quad (\text{A2.1.2})$$

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

Example: Adsorption of 3-methylthiophene in isooctane on NiX zeolite (solution : adsorbent = 200) at room temperature

From the calibration of sulfur compounds:

Respond factor of component i (RMR_i)

$$\text{RMR of 3-methylthiophene} = 0.753$$

Respond factor of standard component (RMR_{std})

$$\text{RMR of isooctane} = 1$$

Initial concentration

$$\text{Peak area of 3-MT1 } (A_{3-MT(1)}) = 26021$$

$$\text{Peak area of 3-MT2 } (A_{3-MT(2)}) = 22506$$

$$\text{Peak area of isooctane1 } (A_{std(1)}) = 69072100$$

$$\text{Peak area of isooctane2 } (A_{std(2)}) = 59749900$$

$$\begin{aligned} Y_{3-MT(1)} &= \frac{(26021/0.753)}{(26021/0.753) + (69072100/1)} \\ &= 500.045 * 10^{-6} \\ &= 500.045 \text{ ppmw} \end{aligned}$$

$$\begin{aligned} Y_{3-MT(2)} &= \frac{(22506/0.753)}{(22506/0.753) + (59749900/1)} \\ &= 499.976 * 10^{-6} \\ &= 499.976 \text{ ppmw} \end{aligned}$$

So, average initial concentration of 3-MT in isooctane

$$\begin{aligned} Y_{3-MT} &= \frac{500.045 + 499.976}{2} \\ &= 500.010 \text{ ppmw} \end{aligned}$$

Concentration of 3-MT after adsorption for 8 hours

$$\text{Peak area of 3-MT1 } (A_{13-MT}) = 11129$$

$$\text{Peak area of 3-MT2 } (A_{23-MT}) = 11644$$

$$\text{Peak area of isooctane1 } (A_{1std}) = 52812300$$

Peak area of isooctane1 ($A_{2_{std}}$) = 55239600

$$\begin{aligned} Y_{3-MT(1)} &= \frac{(11129/0.753)}{(11129/0.753) + (52812300/1)} \\ &= 0.0002797358 * 10^6 \\ &= 279.7358 \text{ ppmw} \end{aligned}$$

$$\begin{aligned} Y_{3-MT(2)} &= \frac{(11644/0.753)}{(11644/0.753) + (55239600/1)} \\ &= 0.0002798563 * 10^6 \\ &= 279.8563 \text{ ppmw} \end{aligned}$$

So, average concentration of 3-MT in isooctane after adsorption

$$\begin{aligned} Y_{3-MT} &= \frac{279.7358 + 279.8563}{2} \\ &= 279.796 \text{ ppmw} \end{aligned}$$

A3 Calculation of amount of adsorption of sulfur compounds (or Benzene) on ion-exchanged zeolite in static adsorption experiment

$$A_i = \frac{F * C_i}{100} - \left[\frac{C_{if}}{100} * \frac{F * (100 - C_i)}{(100 - C_{if})} \right]$$

A_i = Amount of sulfur compound adsorbed on adsorbent

C_i = Concentration of sulfur compound before adsorption (%)

C_f = Concentration of sulfur compound after adsorption (%)

F = Amount of simulated fuels before adsorption (g)

Example: Adsorption of 3-methylthiophene in isooctane on NiX zeolite (solution : adsorbent = 200) at room temperature

Initial concentration of 3-MT (C_{3-MT_i}) = 500.011 ppmw

$$= 500.011 * \frac{100}{1000000}$$

$$= 0.05\%$$

Concentration of 3-MT after adsorption ($C_{3\text{-MT}}$) = 279.796 ppmw

$$= 279.796 * \frac{100}{1000000}$$

$$= 0.0279 \%$$

Amount of simulated fuel = 8.2338 g

$$\text{Thus, } A_{3\text{-MT}} = \frac{8.2338 * 0.05}{100} - \left[\frac{0.0279}{100} * \frac{8.2338 * (100 - 0.05)}{(100 - 0.0279)} \right]$$

$$= 0.0018 \text{ g}$$

Molecular weight of 3-MT = 98.1624 g/gmol

$$A_{3\text{-MT}} = \frac{0.0018}{98.162} * 1000$$

$$= 0.0185 \text{ mmol}$$

Amount of adsorbent (Ni-13X) = 0.0971 g

Therefore, the amount of 3-methylthiophene adsorbed on NiX zeolite = $\frac{0.0185}{0.0971}$

$$= 0.1903 \text{ mmol/g-sorbent}$$

A4 Calculation of amount of adsorption of sulfur compounds (or Toluene) on ion-exchanged zeolite in dynamic adsorption experiment

A4.1 Dead-volume of fixed bed reactor

To find out the Dead-volume of fixed bed reactor, the breakthrough curve of model fuel (isooctane and 1wt % of toluene) without adsorbent was performed in this study. By applying First Moment of the Breakthrough Curve (μ), we can determine the Dead volume:

$$\mu_1 = \mu = \int_0^{\infty} (1 - y) dV \quad y = \frac{c(V)}{c_0}$$

Where μ : mean breakthrough volume

C: concentration of sulfur compounds in the feed (mole or g)

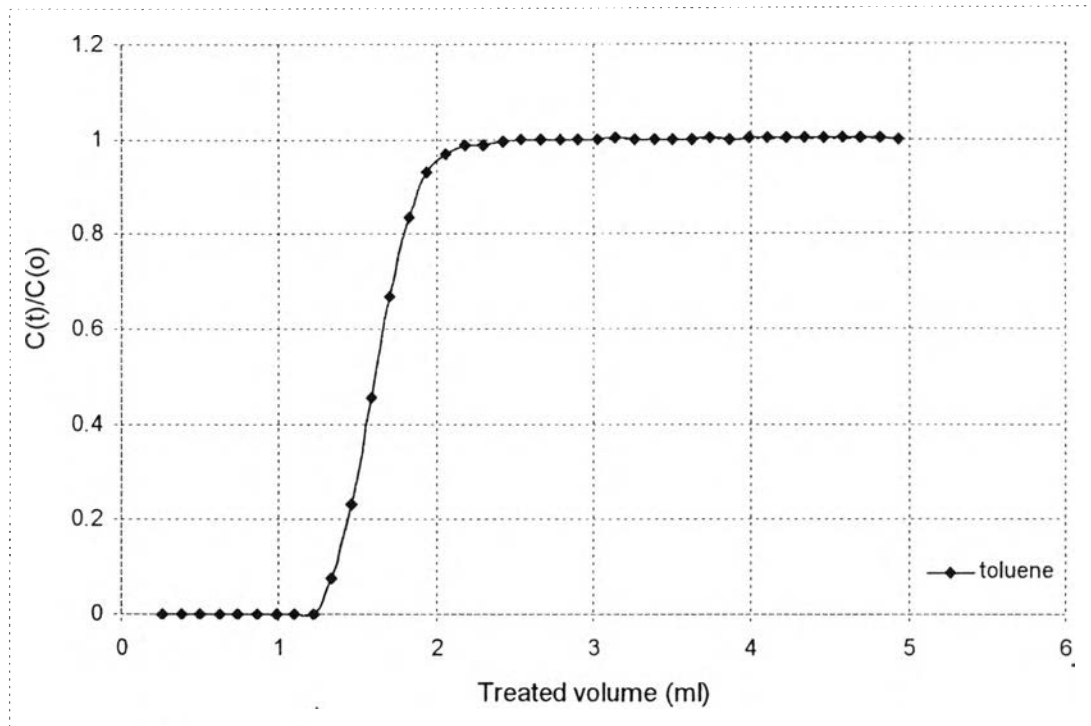


Figure A1. Breakthrough curve without adsorbent.

Hence, Dead-volume = $\mu = 1.62$ ml

A4.2 Amount of adsorption of sulfur compounds (or Toluene) on ion-exchanged zeolite in dynamic adsorption experiment

Example: Adsorption of 3-methylthiophene in model fuels of isooctane, ~ 400 ppmw sulfur content and 1% by weight of toluene on NiY zeolite

Setting parameter of breakthrough adsorption experiment:

Number of the collected vials=	60
Collected time	= 0.36 min
Waste time	= 0.3 min
Wait time	= 1.89 min
F (Flow rate)	= 5 ml/min
Dead-volume	= 1.62 ml
Diameter of grain	= 0.7 mm
Structural density (ρ_s)	= 1.895 g/cm ³
Macroporous volume (v_M)	= 0.36 cm ³ /g

Microporous volume (v_{μ})	= 0.231 cm ³ /g
Mass of adsorbent	= 6.96 g
Density of fuel	= 0.692
Particle density (ρ_P)	= 0.999 g/cm ³
Bulk density (ρ_B)	= 0.714 g/cm ³
C_o (3-MT)	= 370 ppm
C_o (Toluene)	= 1%
T_a	= Waste time + Wait time/2 = 1.245 min
T_p	= Totally time / Numbers of vials = 2.25 min
u (superficial liquid velocity in empty column (cm/min))	= ratio flow rate / column section = 12.992 min
Particle porosity (ϵ_p)	= Partical density * V_M = 0.359
Interparticle porosity (ϵ_i)	= 1- (ρ_B/ ρ_P) = 0.29
Total Macroporous volume (V_M)	= v_M * Mass of adsorbent = 2.5 cm ³
Total Microporous volume (V_{μ})	= v_{μ} * Mass of adsorbent = 2.78 cm ³
Total Macroporous and Microporous volume	= $V_M + V_{\mu}$ = 5.28 cm ³
Total Macroporous and Microporous volume_exp (> Total Macroporous and Microporous volume)	= 7 cm ³
Total Bed porosity (ϵ_B)	= Total Macroporous and Microporous volume_exp/ Volume of column = 0.72
At the Collected Vial No.i:	
Average time	= $T_a + (i-1/2) * T_p$

$$\begin{aligned} \text{Average volume of fuel} &= T_a * F + (i-1/2) * T_p * F \\ \text{Amount of treated volume} &= \text{Average volume of fuel} - \text{Dead-volume} \end{aligned}$$

Hence, Cumulative effluent volume of 3-MT = $\mu = 193.44$ ml

$$= 193.44 / \text{mass of adsorbent} = 29.9 \text{ (ml/g-zeolite)}$$

$$\text{Mass of Cumulative effluent volume of 3-MT} = \mu * d = 133.86 \text{ (g)}$$

$$\text{Amount of 3-MT in the comlume} = \mu * d * C_o = 0.05 \text{ (g)}$$

$$\begin{aligned} \text{Amount of 3-MT adsorbed} &= \text{Amount of 3-MT in the comlume} * (1 - \epsilon_B) \\ &= 0.014 \text{ (g)} = 0.014 * 1000 / \text{mass of adsorbent} = 2.15 \text{ (mg/g-zeolite)} \\ &= 2.15 / \text{Molecular weight of 3-MT} = 0.0219 \text{ (mmole/g-zeolite)} \end{aligned}$$

$$\text{Cumulative effluent volume of Toluene} = \mu = 110.36 \text{ ml}$$

$$= 110.36 / \text{mass of adsorbent} = 17.08 \text{ (ml/g-zeolite)}$$

$$\text{Mass of Cumulative effluent volume of Toluene} = \mu * d = 76.36 \text{ (g)}$$

$$\text{Amount of Toluene in the comlume} = \mu * d * C_o = 0.82 \text{ (g)}$$

$$\begin{aligned} \text{Amount of Toluene adsorbed} &= \text{Amount of Toluene in the comlume} * (1 - \epsilon_B) \\ &= 0.232 \text{ (g)} = 0.232 * 1000 / \text{mass of adsorbent} = 36 \text{ (mg/g-zeolite)} \\ &= 36 / \text{Molecular weight of Toluene} = 0.3911 \text{ (mmole/g-zeolite)} \end{aligned}$$

$$\text{Henry's constant of 3-MT} = \text{Amount of 3-MT adsorbed} / C_o \text{ (3-MT)} = 8.44$$

$$\begin{aligned} \text{Henry's constant of Toluene} &= \text{Amount of Toluene adsorbed} / C_o \text{ (Toluene)} \\ &= 8.44 \end{aligned}$$

$$\text{Selectivity of 3-MT over toluene} = \alpha_{Sul/Tol} = \frac{q_{Sul} / C_{Sul}}{q_{Tol} / C_{Tol}} = 1.75$$

A4.3 Concentration of soluble water in 700g model fuels

Dependence of the Solubility of Water on Hydrocarbon equation

(Constantine Tsionopoulos, 2001) was applied:

$$\ln x_w = \frac{-79.6677 - 6.6547CN}{9.5470 + CN}$$

Where x_w : The solubility of water in hydrocarbon at 298K

CN: Carbon number

With isooctane used as model fuel: CN = 8

$$\ln x_w = \frac{-79.6677 - 6.6547 * 8}{9.5470 + 8} = -7.5572$$

$$x_w = 0.000522$$

$$\text{Moles of isooctane} = 700/114 = 6.14 \text{ mol}$$

$$\text{Moles of soluble water in model fuels} = 6.14 \times 0.000522 = 0.0032 \text{ mol}$$

$$\text{Amount of soluble water in model fuels} = 0.0032 \times 18 = 0.0577 \text{ g}$$

$$\text{Concentration of soluble water in fuels} = \frac{0.0577 \times 100}{700} = 0.00824\% = 82.4 \text{ ppm}$$

APPENDIX B Experimental data

Table B1 Effect of temperature on metal loading on NaX and NaY zeolites

NaX zeolite

Temperature	Concentration of Ni ²⁺ in zeolite (µg/ml)	Times of dilution (times)	Concentration before dilution (µg/ml)	Amount of Ni ²⁺ (g)	Amount of sorbent (g)	%Wt
Room temp.	3.297	25	82.43	0.00824	0.1208	6.82
45°C	3.732	25	93.31	0.00933	0.1248	7.48
60°C	3.935	25	98.37	0.00984	0.1313	7.49
100°C	3.686	25	92.15	0.00921	0.1215	7.58
135°C	4.339	25	108.48	0.01084	0.1269	8.55
150°C	4.217	25	105.44	0.01054	0.1168	9.02

NaY zeolite

Temperature	Concentration of Ni ²⁺ in zeolite (µg/ml)	Times of dilution (times)	Concentration before dilution (µg/ml)	Amount of Ni ²⁺ (g)	Amount of sorbent (g)	%Wt
Room temp.	2.098	25	52.45	0.00525	0.1060	4.95
45°C	2.250	25	56.26	0.00562	0.1098	5.12
60°C	2.420	25	60.49	0.00605	0.1143	5.29
100°C	2.403	25	60.07	0.00601	0.1130	5.32
135°C	2.606	25	65.14	0.00651	0.1014	6.42
150°C	2.654	25	66.36	0.00664	0.1017	6.53

Table B2 Amount of metal loading on NaX zeolite (at 45°C) and NaY zeolite (at 135°C) with different solution to adsorbent (S/A) in exchanging process

Adsorbent	Concentration of Ni ²⁺ in zeolite (µg/ml)	Times of dilution (times)	Concentration before dilution (µg/ml)	Amount of Ni ²⁺ (g)	Amount of sorbent (g)	%Wt
NaX (S/A=50)	1.229	25	30.73	0.00307	0.117	2.63
NaX (S/A=100)	2.338	25	58.47	0.00584	0.106	5.52
NaX (S/A=200)	2.953	25	73.84	0.00738	0.096	7.67

Adsorbent	Concentration of Ni ²⁺ in zeolite (µg/ml)	Times of dilution (times)	Concentration before dilution (µg/ml)	Amount of Ni ²⁺ (g)	Amount of sorbent (g)	%Wt
NiY (S/A=50)	1.083	25	27.08	0.00271	0.107	2.53
NiY(S/A=100)	2.119	25	52.98	0.00530	0.109	4.86
NiY(S/A=200)	2.606	25	65.14	0.00651	0.101	6.42

Table B3 Ion-exchange isotherm

NaX zeolite

Adsorbent	Metal	Valencies of cation (Z_i)	Concentration of metal in zeolite (n_i) (mmol/ml)	Concentration of metal in solution phase ($n_{i(S)}$) (mmol/ml)	E_A	$E_{A(S)}$
NiX (S/A=50)	Ni ²⁺	+2	0.00052	0.00011	0.244	0.011
	Na ⁺	+1	0.00322	0.01938		
NiX (S/A=100)	Ni ²⁺	+2	0.00094	0.00056	0.468	0.083
	Na ⁺	+1	0.00214	0.01244		
NiX (S/A=200)	Ni ²⁺	+2	0.00159	0.00346	0.700	0.410
	Na ⁺	+1	0.00137	0.00996		

NaY zeolite

Adsorbent	Metal	Valencies of cation (Z_i)	Concentration of metal in zeolite (n_i) (mmol/ml)	Concentration of metal in solution phase ($n_{i(S)}$) (mmol/ml)	E_A	$E_{A(S)}$
NiY (S/A=50)	Ni ²⁺	+2	0.00040	0.00011	0.138	0.006
	Na ⁺	+1	0.00254	0.01740		
NiY (S/A=100)	Ni ²⁺	+2	0.00077	0.00118	0.283	0.054
	Na ⁺	+1	0.00196	0.02066		
NiY (S/A=200)	Ni ²⁺	+2	0.00111	0.00405	0.417	0.157
	Na ⁺	+1	0.00155	0.02175		

Table B4 Adsorption isotherm of 3-methylthiophene in isoctane at room temperature by using NiX zeolite with different solution : adsorbent (S/A) in exchanging process (fuel: adsorbent = 85)

Adsorbent	Initial concentration (ppmw)	%C _i	Final concentration (ppmw)	%C _f	Equilibrium concentration (mmol-S/g-fuel)	Solution weight (g)	Adsorbent weight (g)	Adsorbed 3-MT (mmol-S/g-sorbent)
NiX (S/A=50)	500.010	0.050	279.790	0.028	2.85030	8.2338	0.0971	0.1903
	1000.14	0.100	598.540	0.060	6.09740	7.9353	0.0935	0.3474
	1500.11	0.150	945.270	0.095	9.62970	8.6486	0.1012	0.4835
	1998.87	0.199	1264.12	0.126	12.8779	8.4528	0.0998	0.6348
	2498.93	0.249	1579.99	0.158	16.0957	9.1114	0.1082	0.7896
NiX (S/A=100)	500.010	0.050	281.230	0.028	2.86490	8.5775	0.1012	0.1890
	1000.14	0.100	617.190	0.062	6.28750	8.5653	0.1000	0.3343
	1500.11	0.150	856.000	0.086	8.72020	9.4761	0.1250	0.4979
	1998.87	0.199	1266.45	0.127	12.9016	8.2184	0.1025	0.5990
	2498.93	0.249	1636.80	0.164	16.6744	10.302	0.1231	0.7362
NiX (S/A=200)	497.920	0.047	259.510	0.026	2.64370	13.619	0.1622	0.1881
	1005.13	0.100	582.500	0.058	5.93410	6.9810	0.0816	0.3686
	1486.06	0.148	871.430	0.087	8.87750	12.215	0.1528	0.5010
	2082.60	0.208	1327.03	0.132	13.5188	7.5304	0.0887	0.6543
	2498.58	0.249	1651.32	0.165	16.8224	9.1798	0.1048	0.7573
NaX	500.010	0.050	273.850	0.027	2.78970	16.859	0.2000	0.1943
	1000.14	0.100	558.940	0.056	5.69400	14.471	0.1733	0.3755
	1500.11	0.150	930.770	0.093	9.48190	9.9831	0.1116	0.5194
	1998.87	0.199	1223.08	0.122	12.4597	12.065	0.1462	0.6530
	2498.93	0.249	1692.31	0.169	17.2399	9.4599	0.1125	0.6904

Table B5 Adsorption isotherm of benzothiophene in isooctane at room temperature by using NiX zeolite with different solution : adsorbent (S/A) in exchanging process (fuel: adsorbent = 85)

Adsorbent	Initial concentration (ppmw)	%C _i	Final concentration (ppmw)	%C _f	Equilibrium concentration (μmol-S/g-fuel)	Solution weight (g)	Adsorbent weight (g)	Adsorbed BT (mmol-S/g-sorbent)
NiX (S/A=50)	513.560	0.051	77.610	0.008	0.5783	10.354	0.1212	0.2776
	963.960	0.096	185.82	0.019	1.3847	10.364	0.1221	0.4923
	1414.76	0.141	375.08	0.038	2.7950	9.5126	0.1118	0.6595
	2098.07	0.210	775.47	0.078	5.7786	6.7982	0.0800	0.8382
	2536.77	0.254	1101.3	0.110	8.2069	5.7257	0.0674	0.9097
NiX (S/A=100)	513.560	0.051	82.900	0.008	0.6177	10.551	0.1241	0.2729
	963.960	0.096	192.96	0.019	1.4379	9.8174	0.1155	0.4884
	1414.76	0.141	394.11	0.039	2.9368	10.602	0.1227	0.6574
	2098.07	0.210	805.53	0.081	6.0027	9.938	0.1166	0.8216
	2536.77	0.254	1172.6	0.117	8.7381	10.391	0.1222	0.8654
NiX (S/A=200)	513.560	0.051	89.030	0.009	0.6634	10.333	0.1216	0.2688
	963.960	0.096	209.06	0.021	1.5579	10.078	0.1182	0.4797
	1414.76	0.141	406.59	0.041	3.0298	10.372	0.122	0.6390
	2098.07	0.210	816.51	0.082	6.0845	11.764	0.1385	0.8118
	2536.77	0.254	1167.5	0.117	8.7000	10.118	0.1190	0.8686
NaX	513.560	0.051	64.560	0.006	0.4811	10.149	0.1194	0.2844
	963.960	0.096	187.46	0.019	1.3969	10.443	0.1226	0.4930
	1414.76	0.141	414.65	0.041	3.0899	10.004	0.1177	0.6337
	2098.07	0.210	832.09	0.083	6.2006	10.151	0.1195	0.8020
	2536.77	0.254	1149.2	0.115	8.5637	10.175	0.1197	0.8800

Table B6 Adsorption isotherm of 3-methylthiophene in benzene at room temperature by using NiX zeolite with different solution : adsorbent (S/A) in exchanging process (fuel: adsorbent = 85)

Adsorbent	Initial concentration (ppmw)	%C _i	Final concentration (ppmw)	%C _f	Equilibrium concentration (μmol-S/g-fuel)	Solution weight (g)	Adsorbent weight (g)	Adsorbed 3-MT (mmol-S/g-sorbent)
NiX (S/A=50)	505.330	0.051	481.950	0.048	4.90980	13.843	0.1629	0.0202
	1035.56	0.104	989.860	0.099	10.0839	9.0858	0.1082	0.0391
	1497.49	0.150	1438.89	0.144	14.6583	10.075	0.1190	0.0507
	1997.50	0.200	1925.12	0.193	19.6116	10.319	0.1300	0.0588
	2506.09	0.251	2423.38	0.242	24.6875	10.119	0.1185	0.0721
NiX (S/A=100)	505.330	0.051	489.340	0.049	4.98500	10.100	0.1174	0.0140
	1035.56	0.104	1004.30	0.100	10.2310	10.310	0.1273	0.0258
	1497.49	0.150	1450.34	0.145	14.7749	10.366	0.1431	0.0349
	1997.50	0.200	1949.13	0.195	19.8561	9.2900	0.1100	0.0417
	2506.09	0.251	2449.71	0.245	24.9557	9.3640	0.1126	0.0479
NiX (S/A=200)	505.330	0.051	489.930	0.049	4.99100	11.250	0.1323	0.0133
	1035.56	0.104	1002.53	0.100	10.2130	7.8190	0.0977	0.0270
	1497.49	0.150	1457.68	0.146	14.8497	8.6020	0.1045	0.0334
	1997.50	0.200	1952.00	0.195	19.8854	10.520	0.1259	0.0388
	2506.09	0.251	2454.68	0.245	25.0063	9.7720	0.1165	0.0440
NaX	505.330	0.051	483.360	0.048	4.92410	7.2990	0.0852	0.0192
	1035.56	0.104	992.290	0.099	10.1086	8.4470	0.0994	0.0375
	1497.49	0.150	1441.16	0.144	14.6813	8.4490	0.0963	0.0504
	1997.50	0.200	1950.53	0.195	19.8705	10.520	0.0939	0.0537
	2506.09	0.251	2437.41	0.244	24.8303	8.5600	0.1036	0.0580

Table B7 Adsorption isotherm of benzothiophene in benzene at room temperature by using NiX zeolite with different solution : adsorbent (S/A) in exchanging process (fuel: adsorbent = 85)

Adsorbent	Initial concentration (ppmw)	%C _i	Final concentration (ppmw)	%C _f	Equilibrium concentration (mmol-S/g-fuel)	Solution weight (g)	Adsorbent weight (g)	Adsorbed BT (mmol-S/g-sorbent)
NiX (S/A=50)	517.220	0.052	484.570	0.048	3.61090	8.5423	0.1007	0.0206
	989.990	0.099	933.420	0.093	6.95570	9.4730	0.1110	0.0360
	1478.98	0.148	1398.65	0.140	10.4225	9.4271	0.1108	0.0510
	1980.49	0.198	1888.72	0.189	14.0744	10.167	0.1135	0.0614
	2495.80	0.250	2389.46	0.239	17.8059	9.7010	0.1141	0.0675
NiX (S/A=100)	517.220	0.052	486.980	0.049	3.62890	9.8571	0.1156	0.0192
	989.990	0.099	941.400	0.094	7.01520	9.9106	0.1167	0.0308
	1478.98	0.148	1408.21	0.141	10.4937	10.803	0.1271	0.0449
	1980.49	0.198	1891.88	0.189	14.0980	9.9742	0.1172	0.0563
	2495.80	0.250	2397.55	0.240	17.8662	8.6140	0.1013	0.0624
NiX (S/A=200)	517.220	0.052	491.730	0.049	3.66430	11.057	0.1301	0.0161
	989.990	0.099	943.890	0.094	7.03370	9.5955	0.1129	0.0292
	1478.98	0.148	1416.27	0.142	10.5539	9.3739	0.1102	0.0398
	1980.49	0.198	1907.89	0.191	14.2173	10.031	0.1180	0.0461
	2495.80	0.250	2403.22	0.240	17.9084	8.6812	0.1117	0.0537
NaX	517.220	0.052	494.300	0.049	3.68340	10.269	0.1208	0.0145
	989.990	0.099	948.810	0.095	7.07040	10.758	0.1264	0.0261
	1478.98	0.148	1419.30	0.142	10.5764	10.161	0.1195	0.0379
	1980.49	0.198	1911.41	0.191	14.2435	8.6812	0.1020	0.0439
	2495.80	0.250	2423.37	0.242	18.0586	9.8510	0.1158	0.0460

Table B8 Adsorption of 3-MT and Benzene on NiX (7.48%wt Ni) and NaX zeolites in ternary system (fuel: adsorbent = 85)

Adsorbent	Initial conc. of C ₆ H ₆ (ppmw)	%C _i	Final conc. of C ₆ H ₆ (ppmw)	%C _f	Initial conc. of 3-MT (ppmw)	%C _i	Final conc. of 3-MT (ppmw)	%C _f	Solution weight (g)	Adsorbent weight (g)	Adsorbed 3-MT (mmol-S/g-sorbent)	Adsorbed C ₆ H ₆ (mmol-S/g-sorbent)
NiX (7.48%wt Ni)	10283.05	1.028	10140.39	1.014	2020.02	0.202	1481.83	0.148	10.0387	0.112	0.4921	0.1656
	20013.20	2.001	19795.53	1.980	2000.19	0.200	1596.89	0.160	10.1364	0.115	0.3643	0.2520
	30776.95	3.078	30333.19	3.033	2042.64	0.204	1845.77	0.185	10.0203	0.116	0.1733	0.5060
	60093.99	6.009	59592.51	5.959	2028.55	0.203	1899.66	0.190	10.0121	0.122	0.1079	0.5606
	89967.32	8.997	89508.95	8.951	2083.02	0.208	1969.93	0.197	10.0697	0.118	0.0983	0.5494
	120925.64	12.090	120451.03	12.045	2054.34	0.205	1945.29	0.195	10.3267	0.121	0.0947	0.5885
	150223.75	15.022	149772.04	14.977	2010.90	0.201	1907.39	0.191	10.2157	0.119	0.0907	0.5847
NaX	10283.05	1.030	10048.127	1.005	2031.56	0.203	1650.17	0.165	10.0023	0.102	0.3805	0.2975
	20013.20	2.001	19608.263	1.961	2018.40	0.202	1794.97	0.179	10.0460	0.111	0.2056	0.4775
	30776.95	3.080	30291.674	3.029	2042.64	0.204	1873.02	0.187	10.0548	0.116	0.1501	0.5561
	60093.99	6.010	59594.556	5.959	2028.55	0.203	1931.29	0.193	10.0150	0.115	0.0865	0.5935
	89967.32	9.000	89468.980	8.947	2083.02	0.208	1995.04	0.200	10.0130	0.116	0.0777	0.6067
	120925.64	12.090	120435.508	12.044	2054.34	0.205	1969.28	0.197	9.9770	0.117	0.0738	0.6071
	150223.75	15.020	149728.204	14.973	2010.90	0.201	1924.28	0.192	9.8184	0.116	0.0752	0.6352

Table B9 Adsorption of BT and Benzene on NiX (7.48%wt Ni) and NaX zeolites in ternary system (fuel: adsorbent = 85)

Adsorbent	Initial conc. of C ₆ H ₆ (ppmw)	%C _i	Final conc. of C ₆ H ₆ (ppmw)	%C _f	Initial conc. of BT (ppmw)	%C _i	Final conc. of BT (ppmw)	%C _f	Solution weight (g)	Adsorbent weight (g)	Adsorbed BT (mmol-S/g-sorbent)	Adsorbed C ₆ H ₆ (mmol-S/g-sorbent)
NiX (7.48%wt Ni)	10028.23	1.003	9898.79	0.990	1995.82	0.200	983.49	0.098	9.7123	0.1123	0.6531	0.1450
	20011.54	2.001	19716.33	1.972	2008.95	0.201	1290.88	0.129	9.7538	0.1076	0.4857	0.3500
	29745.88	2.975	29322.23	2.932	1960.29	0.196	1408.08	0.141	9.7004	0.1141	0.3503	0.4754
	56971.90	5.697	56372.45	5.637	1992.43	0.199	1756.07	0.176	9.7859	0.1149	0.1503	0.6947
	81918.14	8.192	81329.32	8.133	2002.18	0.200	1862.42	0.186	10.9325	0.1282	0.0890	0.7017
	107421.89	10.742	106793.01	10.679	2085.12	0.209	1974.88	0.197	8.8934	0.1046	0.0700	0.7678
	131741.06	13.174	131143.67	13.114	1960.16	0.196	1857.19	0.186	9.0818	0.1068	0.0654	0.7504
NaX	10028.23	1.003	9782.911	0.9783	1995.82	0.200	1163.29	0.116	9.7125	0.1134	0.5320	0.2720
	20011.54	2.001	19688.882	1.9689	2008.95	0.201	1391.88	0.139	9.7548	0.1176	0.3818	0.4220
	29745.88	2.98	29284.91	2.928	1960.29	0.196	1490.75	0.149	8.8487	0.1041	0.2979	0.5175
	56971.90	5.697	56423.42	5.642	1992.43	0.199	1765.48	0.177	9.9143	0.1166	0.1441	0.6337
	81918.14	8.192	81313.34	8.131	2002.18	0.200	1884.44	0.188	8.6901	0.1022	0.0747	0.7177
	107421.89	10.742	106695.11	10.670	2085.12	0.209	1995.37	0.200	8.5962	0.1205	0.0478	0.7441
	131741.06	13.174	131155.84	13.116	1960.16	0.196	1890.28	0.189	10.2458	0.1155	0.0463	0.7660

Table B10 Adsorption isotherm of 3-methylthiophene in isooctane at room temperature by using NiY zeolite with different exchanged techniques (fuel: adsorbent = 85)

Adsorbent	Initial concentration (ppmw)	%C _i	Final concentration (ppmw)	%C _f	Equilibrium concentration (μmol-S/g-fuel)	Solution weight (g)	Adsorbent weight (g)	Adsorbed 3-MT (mmol-S/g-sorbent)
NiY-SSIE	498.40	0.050	197.64	0.020	2.0134	10.1540	0.1193	0.2608
	1003.76	0.100	415.93	0.042	4.2372	9.8028	0.1153	0.5093
	1504.42	0.150	663.65	0.066	6.7607	9.3670	0.1102	0.7285
	1994.77	0.199	972.28	0.097	9.9048	10.2905	0.1210	0.8867
	2493.88	0.249	1298.90	0.130	13.2322	10.3492	0.1217	1.0366
NiY-LPIE	498.40	0.050	303.33	0.030	3.0901	9.8954	0.1164	0.1690
	1003.76	0.100	656.98	0.066	6.6928	10.0840	0.1187	0.3003
	1504.42	0.150	976.64	0.098	9.9492	9.3670	0.1212	0.4159
	1994.77	0.199	1393.93	0.139	14.2002	10.2905	0.1213	0.5200
	2493.88	0.249	1702.51	0.170	17.3438	10.3492	0.1371	0.6096
NaY	498.40	0.050	291.34	0.029	2.9679	10.2321	0.1231	0.1754
	1003.76	0.100	615.87	0.062	6.2740	9.8543	0.1159	0.3362
	1504.42	0.150	985.38	0.099	10.0383	9.7654	0.115	0.4494
	1994.77	0.199	1361.29	0.136	13.8678	10.2147	0.1209	0.5460
	2493.88	0.249	1835.41	0.184	18.6977	10.0087	0.1178	0.5710

Table B11 Adsorption isotherm of Benzothiophene in isoctane at room temperature by using NiY zeolite with different exchanged techniques (fuel: adsorbent = 85)

Adsorbent	Initial concentration (ppmw)	%C _i	Final concentration (ppmw)	%C _f	Equilibrium concentration (μmol-S/g-fuel)	Solution weight (g)	Adsorbent weight (g)	Adsorbed BT (mmol-S/g-sorbent)
NiY-SSIE	494.56	0.049	48.56	0.005	0.3618	9.6523	0.1136	0.2824
	978.42	0.098	129.47	0.013	0.9648	9.7853	0.1151	0.5379
	1536.51	0.154	296.97	0.030	2.2130	9.6085	0.113	0.7856
	2005.06	0.201	501.47	0.050	3.7369	10.5941	0.1246	0.9531
	2517.95	0.252	767.63	0.077	5.7202	9.8855	0.1163	1.1095
NiY-LPIE	494.56	0.049	90.83	0.009	0.6768	10.6458	0.1252	0.2558
	978.42	0.098	206.22	0.021	1.5367	10.4635	0.1231	0.4892
	1536.51	0.154	484.77	0.048	3.6124	10.2844	0.121	0.6665
	2005.06	0.201	835.05	0.084	6.2226	10.8300	0.1275	0.7412
	2517.95	0.252	1242.43	0.124	9.2584	9.5732	0.1127	0.8084
NaY	494.56	0.049	85.27	0.009	0.6354	13.5414	0.1593	0.2593
	978.42	0.098	255.74	0.026	1.9057	10.5296	0.1237	0.4585
	1536.51	0.154	532.51	0.053	3.9682	12.5264	0.1471	0.6374
	2005.06	0.201	877.95	0.088	6.5424	9.7389	0.1144	0.7156
	2517.95	0.252	1341.58	0.134	9.9972	11.1759	0.1314	0.7466

Table B12 Adsorption isotherm of 3-methylthiophene in benzene at room temperature by using NiY zeolite with different exchanged techniques (fuel: adsorbent = 85)

Adsorbent	Initial concentration (ppmw)	%C _i	Final concentration (ppmw)	%C _f	Equilibrium concentration (μmol-S/g-fuel)	Solution weight (g)	Adsorbent weight (g)	Adsorbed 3-MT (mmol-S/g-sorbent)
NiY-SSIE	492.19	0.049	460.21	0.046	4.6883	10.7327	0.1262	0.0277
	1018.07	0.102	952.55	0.095	9.7038	9.8768	0.1162	0.0568
	1466.43	0.147	1386.81	0.139	14.1277	10.0302	0.1178	0.0692
	2043.58	0.204	1945.57	0.195	19.8199	9.1909	0.1079	0.0852
	2493.21	0.249	2385.47	0.239	24.3013	9.7022	0.1141	0.0936
NiY-LPIE	492.19	0.049	465.96	0.047	4.7468	10.5543	0.1241	0.0227
	1018.07	0.102	969.10	0.097	9.8725	10.3221	0.1214	0.0425
	1466.43	0.147	1402.18	0.140	14.2843	10.1379	0.1191	0.0558
	2043.58	0.204	1964.16	0.196	20.0093	10.4555	0.123	0.0689
	2493.21	0.249	2411.61	0.241	24.5675	10.5301	0.1237	0.0709
NaY	492.19	0.049	469.26	0.047	4.7805	12.5443	0.1475	0.0199
	1018.07	0.102	977.74	0.098	9.9605	9.6156	0.1131	0.0350
	1466.43	0.147	1408.08	0.141	14.3444	9.5382	0.1121	0.0506
	2043.58	0.204	1975.61	0.198	20.1259	10.0038	0.1176	0.0590
	2493.21	0.249	2424.57	0.242	24.6995	9.2155	0.1084	0.0596

Table B13 Adsorption isotherm of Benzothiophene in benzene at room temperature by using NiY zeolite with different exchanged techniques (fuel: adsorbent = 85)

Adsorbent	Initial concentration (ppmw)	%C _i	Final concentration (ppmw)	%C _f	Equilibrium concentration (μmol-S/g-fuel)	Solution weight (g)	Adsorbent weight (g)	Adsorbed BT (mmol-S/g-sorbent)
NiY-SSIE	505.73	0.051	445.54	0.045	2.3201	11.4536	0.1347	0.0382
	1020.26	0.102	909.69	0.091	6.7789	10.9881	0.1292	0.0701
	1489.47	0.149	1337.48	0.134	9.9667	9.3840	0.11	0.0967
	1917.73	0.192	1745.71	0.175	13.0088	9.9412	0.117	0.1091
	2536.81	0.254	2349.27	0.235	17.5064	11.2633	0.1325	0.1191
NiY-LPIE	505.73	0.051	477.04	0.048	3.5548	11.4100	0.1342	0.0182
	1020.26	0.102	965.38	0.097	7.1939	10.1341	0.1191	0.0348
	1489.47	0.149	1416.91	0.142	10.5586	12.0116	0.1414	0.0460
	1917.73	0.192	1839.63	0.184	13.7086	9.4928	0.1116	0.0496
	2536.81	0.254	2450.37	0.245	18.2597	10.9445	0.1285	0.0550
NaY	505.73	0.051	483.54	0.048	3.6033	11.4958	0.1346	0.0141
	1020.26	0.102	977.99	0.098	7.2878	9.3476	0.1098	0.0268
	1489.47	0.149	1433.62	0.143	10.6831	10.9345	0.1287	0.0354
	1917.73	0.192	1849.99	0.185	13.7859	10.1424	0.1192	0.0430
	2536.81	0.254	2465.00	0.246	18.3688	10.9918	0.1286	0.0459

Table B14 Breakthrough curve for the adsorptive removal of 3-MT and Toluene on NaY zeolite

Time (min)	Cumulative effluent volume (ml/g-zeolite)	C(t) of Toluene (%)	C(t) of 3-MT (%)	C(t)/C ₀ of Toluene	C(t)/C ₀ of 3-MT
2.37	1.586	0.000	0.000	0.000	0.000
4.62	3.330	0.000	0.000	0.000	0.000
6.87	5.074	0.000	0.000	0.000	0.000
9.12	6.818	0.000	0.000	0.000	0.000
11.37	8.562	0.000	0.000	0.000	0.000
13.62	10.306	0.000	0.000	0.000	0.000
15.87	12.051	0.000	0.000	0.000	0.000
18.12	13.795	0.044	0.000	0.040	0.000
20.37	15.539	0.098	0.000	0.089	0.000
22.62	17.283	0.175	0.024	0.160	0.625
24.87	19.027	0.275	0.033	0.252	0.850
27.12	20.772	0.394	0.041	0.360	1.070
29.37	22.516	0.511	0.048	0.467	1.227
31.62	24.260	0.620	0.052	0.567	1.336
33.87	26.004	0.715	0.055	0.654	1.408
36.12	27.748	0.802	0.056	0.733	1.444
38.37	29.493	0.874	0.055	0.800	1.416
40.62	31.237	0.935	0.055	0.855	1.411
42.87	32.981	0.978	0.053	0.894	1.359
45.12	34.725	1.013	0.051	0.926	1.307
47.37	36.469	1.034	0.048	0.945	1.248
49.62	38.213	1.051	0.046	0.962	1.191
51.87	39.958	1.064	0.044	0.973	1.134
54.12	41.702	1.072	0.042	0.981	1.095
56.37	43.446	1.077	0.042	0.985	1.080
58.62	45.190	1.080	0.041	0.988	1.049
60.87	46.934	1.084	0.040	0.992	1.021
63.12	48.679	1.088	0.040	0.995	1.023
65.37	50.423	1.091	0.039	0.998	1.013
67.62	52.167	1.090	0.039	0.997	1.010

Note: Flow rate = 5 ml/min

Mass of adsorbent = 6.45 g

Initial concentration of 3-MT = 390 ppmw

Initial concentration of Toluene = 1.093 %

Table B15 Breakthrough curve for the adsorptive removal of 3-MT and Toluene on NiY zeolite

Time (min)	Cumulative effluent volume (ml/g-zeolite)	C(t) of Toluene (%)	C(t) of 3-MT (%)	C(t)/C ₀ of Toluene	C(t)/C ₀ of 3-MT
2.37	1.470	0.000	0.000	0.000	0.000
4.62	3.086	0.000	0.000	0.000	0.000
6.87	4.703	0.000	0.000	0.000	0.000
9.12	6.319	0.008	0.000	0.007	0.000
11.37	7.935	0.024	0.000	0.022	0.000
13.62	9.552	0.059	0.000	0.055	0.000
15.87	11.168	0.126	0.000	0.117	0.000
18.12	12.784	0.242	0.000	0.224	0.000
20.37	14.401	0.410	0.007	0.380	0.191
22.62	16.017	0.596	0.011	0.552	0.300
24.87	17.634	0.760	0.015	0.704	0.408
27.12	19.250	0.891	0.019	0.826	0.517
29.37	20.866	0.983	0.022	0.911	0.599
31.62	22.483	1.036	0.025	0.960	0.681
33.87	24.099	1.066	0.027	0.988	0.735
36.12	25.716	1.081	0.029	1.002	0.790
38.37	27.332	1.079	0.031	1.000	0.844
40.62	28.948	1.079	0.032	1.000	0.871
42.87	30.565	1.082	0.033	1.003	0.899
45.12	32.181	1.075	0.034	0.996	0.926
47.37	33.797	1.080	0.035	1.001	0.953
49.62	35.414	1.079	0.035	1.000	0.953
51.87	37.030	1.079	0.035	1.000	0.953
54.12	38.647	1.083	0.036	1.004	0.980
56.37	40.263	1.078	0.036	0.999	0.980
58.62	41.879	1.076	0.036	0.997	0.980
60.87	43.496	1.081	0.036	1.002	0.980
63.12	45.112	1.080	0.036	1.001	0.980
65.37	46.728	1.075	0.036	0.996	0.980
67.62	48.345	1.078	0.037	0.999	1.007

Note: Flow rate = 5 ml/min
 Mass of adsorbent = 6.45 g
 Initial concentration of 3-MT = 370 ppmw
 Initial concentration of Toluene = 1.079 %

Table B16 Breakthrough curve for the adsorptive removal of 3-MT and Toluene on Cu^(II)Y zeolite

Time (min)	Cumulative effluent volume (ml/g-zeolite)	C(t) of Toluene (%)	C(t) of 3-MT (%)	C(t)/C ₀ of Toluene	C(t)/C ₀ of 3-MT
3.120	2.219	0.000	0.000	0.000	0.000
6.120	4.600	0.007	0.000	0.006	0.000
9.120	6.981	0.031	0.000	0.028	0.000
12.120	9.362	0.079	0.000	0.072	0.000
15.120	11.743	0.169	0.000	0.153	0.000
18.120	14.124	0.330	0.000	0.299	0.000
21.120	16.505	0.530	0.000	0.480	0.000
24.120	18.886	0.732	0.001	0.664	0.028
27.120	21.267	0.889	0.002	0.806	0.057
30.120	23.648	0.983	0.003	0.891	0.085
33.120	26.029	1.037	0.004	0.940	0.114
36.120	28.410	1.069	0.005	0.969	0.142
39.120	30.790	1.085	0.006	0.984	0.171
42.120	33.171	1.092	0.007	0.990	0.199
45.120	35.552	1.103	0.008	1.000	0.228
48.120	37.933	1.107	0.009	1.003	0.256
51.120	40.314	1.104	0.010	1.001	0.284
54.120	42.695	1.114	0.012	1.010	0.341
57.120	45.076	1.115	0.013	1.011	0.370
60.120	47.457	1.111	0.014	1.007	0.398
63.120	49.838	1.115	0.015	1.011	0.427
66.120	52.219	1.109	0.017	1.005	0.484
69.120	54.600	1.100	0.018	0.997	0.512
72.120	56.981	1.100	0.019	0.997	0.540
75.120	59.362	1.104	0.020	1.001	0.569
78.120	61.743	1.100	0.021	0.997	0.597
81.120	64.124	1.100	0.022	0.997	0.626
84.120	66.505	1.106	0.023	1.003	0.654
87.120	68.886	1.104	0.023	1.001	0.654
90.120	71.267	1.101	0.024	0.998	0.683

Note: Flow rate = 5 ml/min

Mass of adsorbent = 6.45 g

Initial concentration of 3-MT = 350 ppmw

Initial concentration of Toluene = 1.103 %

Table B17 Breakthrough curve for the adsorptive removal of 3-MT and Toluene on NaX zeolite

Time (min)	Cumulative effluent volume (ml/g-zeolite)	$C(t)$ of Toluene (%)	$C(t)$ of 3-MT (%)	$C(t)/C_0$ of Toluene	$C(t)/C_0$ of 3-MT
3.12	2.240	0.000	0.000	0.000	0.000
6.12	4.644	0.000	0.000	0.000	0.000
9.12	7.048	0.000	0.000	0.000	0.000
12.12	9.452	0.000	0.000	0.000	0.000
15.12	11.856	0.000	0.000	0.000	0.000
18.12	14.260	0.018	0.000	0.016	0.000
21.12	16.663	0.123	0.002	0.111	0.041
24.12	19.067	0.362	0.002	0.326	0.058
27.12	21.471	0.602	0.003	0.541	0.091
30.12	23.875	0.781	0.005	0.702	0.146
33.12	26.279	0.916	0.008	0.823	0.220
36.12	28.683	0.999	0.010	0.899	0.267
39.12	31.087	1.060	0.011	0.953	0.314
42.12	33.490	1.094	0.013	0.984	0.361
45.12	35.894	1.111	0.016	0.999	0.430
48.12	38.298	1.120	0.017	1.007	0.468
51.12	40.702	1.126	0.018	1.013	0.496
54.12	43.106	1.126	0.020	1.012	0.545
57.12	45.510	1.124	0.021	1.010	0.578
60.12	47.913	1.122	0.022	1.009	0.600
63.12	50.317	1.122	0.023	1.009	0.644
66.12	52.721	1.119	0.024	1.006	0.672
69.12	55.125	1.122	0.026	1.009	0.705
72.12	57.529	1.119	0.027	1.007	0.741
75.12	59.933	1.119	0.027	1.007	0.744
78.12	62.337	1.120	0.028	1.007	0.782
81.12	64.740	1.117	0.029	1.004	0.810
84.12	67.144	1.115	0.030	1.003	0.815
87.12	69.548	1.118	0.031	1.005	0.845
90.12	71.952	1.113	0.031	1.000	0.862

Note: Flow rate = 5 ml/min
 Mass of adsorbent = 6.45 g
 Initial concentration of 3-MT = 360 ppmw
 Initial concentration of Toluene = 1.112%

Table B18 Breakthrough curve for the adsorptive removal of 3-MT and Toluene on NiX zeolite

Time (min)	Cumulative effluent volume (ml/g-zeolite)	C(t) of Toluene (%)	C(t) of 3-MT (%)	C(t)/C ₀ of Toluene	C(t)/C ₀ of 3-MT
3.12	2.226	0.009	0.000	0.008	0.000
6.12	4.615	0.012	0.000	0.011	0.000
9.12	7.003	0.191	0.000	0.169	0.000
12.12	9.392	0.624	0.001	0.553	0.022
15.12	11.780	0.957	0.005	0.849	0.109
18.12	14.169	1.099	0.008	0.974	0.174
21.12	16.557	1.140	0.013	1.011	0.283
24.12	18.946	1.145	0.018	1.015	0.392
27.12	21.334	1.141	0.023	1.012	0.500
30.12	23.723	1.142	0.028	1.013	0.609
33.12	26.111	1.141	0.031	1.012	0.675
36.12	28.500	1.137	0.035	1.008	0.762
39.12	30.889	1.130	0.037	1.002	0.805
42.12	33.277	1.127	0.039	0.999	0.849
45.12	35.666	1.129	0.041	1.001	0.892
48.12	38.054	1.132	0.042	1.004	0.914
51.12	40.443	1.131	0.043	1.003	0.936
54.12	42.831	1.126	0.044	0.998	0.957
57.12	45.220	1.125	0.044	0.998	0.957
60.12	47.608	1.129	0.045	1.001	0.979
63.12	49.997	1.130	0.045	1.002	0.979
66.12	52.385	1.127	0.045	0.999	0.979
69.12	54.774	1.124	0.045	0.997	0.979
72.12	57.162	1.126	0.046	0.998	1.001
75.12	59.551	1.131	0.046	1.003	1.001
78.12	61.939	1.128	0.046	1.000	1.001
81.12	64.328	1.126	0.046	0.998	1.001
84.12	66.717	1.128	0.046	1.000	1.001
87.12	69.105	1.126	0.046	0.998	1.001
90.12	71.494	1.120	0.046	0.993	1.001

Note: Flow rate = 5 ml/min
 Mass of adsorbent = 6.45 g
 Initial concentration of 3-MT = 460 ppmw
 Initial concentration of Toluene = 1.128 %

Table B19 Breakthrough curve for the adsorptive removal of 3-MT and Toluene on NaY zeolite with pre-adsorbed water

Time (min)	Cumulative effluent volume (ml/g-zeolite)	C(t) of Toluene (%)	C(t) of 3-MT (%)	C(t)/C ₀ of Toluene	C(t)/C ₀ of 3-MT
2.046	1.529	0.000	0.000	0.000	0.000
4.296	3.211	0.000	0.000	0.000	0.000
6.546	4.892	0.000	0.000	0.000	0.000
8.796	6.574	0.000	0.000	0.000	0.000
11.046	8.256	0.021	0.000	0.018	0.000
13.296	9.937	0.059	0.011	0.051	0.208
15.546	11.619	0.135	0.022	0.117	0.417
17.796	13.300	0.258	0.035	0.224	0.663
20.046	14.982	0.410	0.049	0.356	0.929
22.296	16.664	0.570	0.061	0.495	1.156
24.546	18.345	0.707	0.068	0.614	1.289
26.796	20.027	0.831	0.072	0.722	1.364
29.046	21.709	0.931	0.073	0.809	1.383
31.296	23.390	1.002	0.072	0.870	1.364
33.546	25.072	1.051	0.069	0.913	1.308
35.796	26.753	1.084	0.066	0.942	1.251
38.046	28.435	1.110	0.063	0.964	1.194
40.296	30.117	1.105	0.059	0.960	1.118
42.546	31.798	1.131	0.058	0.983	1.099
44.796	33.480	1.141	0.056	0.991	1.061
47.046	35.161	1.140	0.055	0.990	1.042
49.296	36.843	1.147	0.054	0.996	1.023
51.546	38.525	1.151	0.054	1.000	1.023
53.796	40.206	1.150	0.053	0.999	1.004
56.046	41.888	1.145	0.053	0.995	1.004
58.296	43.570	1.151	0.053	1.000	1.004
60.546	45.251	1.153	0.053	1.002	1.004
62.796	46.933	1.149	0.053	0.998	1.004
65.046	48.614	1.151	0.053	1.000	1.004
67.296	50.296	1.151	0.053	1.000	1.004

Note: Flow rate = 5 ml/min

Mass of adsorbent = 6.69 g

Initial concentration of 3-MT = 530 ppmw

Initial concentration of Toluene = 1.151 %

Table B20 Breakthrough curve for the adsorptive removal of 3-MT and Toluene on NiY zeolite with pre-adsorbed water

Time (min)	Cumulative effluent volume (ml/g-zeolite)	C(t) of Toluene (%)	C(t) of 3-MT (%)	C(t)/C ₀ of Toluene	C(t)/C ₀ of 3-MT
2.370	1.529	0.000	0.000	0.000	0.000
4.620	3.211	0.000	0.000	0.000	0.000
6.870	4.892	0.009	0.000	0.009	0.000
9.120	6.574	0.024	0.000	0.023	0.000
11.370	8.256	0.083	0.000	0.079	0.000
13.620	9.937	0.203	0.012	0.194	0.231
15.870	11.619	0.360	0.018	0.345	0.347
18.120	13.300	0.535	0.025	0.512	0.481
20.370	14.982	0.687	0.031	0.658	0.597
22.620	16.664	0.825	0.036	0.790	0.693
24.870	18.345	0.912	0.040	0.873	0.770
27.120	20.027	0.956	0.042	0.915	0.809
29.370	21.709	1.016	0.046	0.973	0.886
31.620	23.390	1.028	0.047	0.984	0.905
33.870	25.072	1.026	0.047	0.982	0.905
36.120	26.753	1.011	0.049	0.990	0.943
38.370	28.435	1.021	0.049	1.007	0.963
40.620	30.117	1.034	0.049	0.999	0.963
42.870	31.798	1.052	0.050	0.993	0.963
45.120	33.480	1.044	0.050	0.977	0.943
47.370	35.161	1.037	0.050	1.009	1.001
49.620	36.843	1.040	0.051	0.968	0.943
51.870	38.525	1.054	0.052	0.996	0.982
54.120	40.206	1.052	0.052	1.007	1.001
56.370	41.888	1.046	0.052	1.001	1.001
58.620	43.570	1.040	0.051	0.996	0.982
60.870	45.251	1.040	0.051	0.998	1.001
63.120	46.933	1.035	0.051	0.996	0.982
65.370	48.614	1.036	0.051	0.999	1.001
67.620	50.296	1.042	0.052	0.991	0.982

Note: Flow rate = 5 ml/min
 Mass of adsorbent = 6.69 g
 Initial concentration of 3-MT = 520 ppmw
 Initial concentration of Toluene = 1.045 %

Table B21 Breakthrough curve for the adsorptive removal of 3-MT and Toluene on Cu^(II)Y zeolite with pre-adsorbed water

Time (min)	Cumulative effluent volume (ml/g-zeolite)	C(t) of Toluene (%)	C(t) of 3-MT (%)	C(t)/C ₀ of Toluene	C(t)/C ₀ of 3-MT
2.796	2.098	0.041	0.000	0.038	0.000
5.796	4.349	0.110	0.000	0.101	0.000
8.796	6.601	0.234	0.000	0.215	0.000
11.796	8.852	0.435	0.004	0.399	0.097
14.796	11.103	0.648	0.008	0.594	0.195
17.796	13.354	0.808	0.010	0.741	0.244
20.796	15.606	0.922	0.011	0.846	0.268
23.796	17.857	0.992	0.013	0.910	0.317
26.796	20.108	1.022	0.014	0.937	0.341
29.796	22.359	1.041	0.015	0.955	0.365
32.796	24.611	1.053	0.017	0.966	0.414
35.796	26.862	1.041	0.018	0.955	0.438
38.796	29.113	1.048	0.019	0.961	0.463
41.796	31.364	1.057	0.021	0.969	0.511
44.796	33.615	1.059	0.022	0.971	0.536
47.796	35.867	1.057	0.023	0.969	0.560
50.796	38.118	1.060	0.023	0.972	0.560
53.796	40.369	1.062	0.026	0.974	0.633
56.796	42.620	1.065	0.026	0.977	0.633
59.796	44.872	1.073	0.028	0.984	0.682
62.796	47.123	1.074	0.028	0.985	0.682
65.796	49.374	1.075	0.029	0.986	0.706
68.796	51.625	1.076	0.029	0.987	0.706
71.796	53.877	1.078	0.031	0.989	0.755
74.796	56.128	1.078	0.032	0.989	0.779
77.796	58.379	1.079	0.033	0.990	0.804
80.796	60.630	1.083	0.033	0.993	0.804
83.796	62.882	1.082	0.033	0.992	0.804
86.796	65.133	1.082	0.034	0.992	0.828
89.796	67.384	1.082	0.034	0.992	0.828

Note: Flow rate = 5 ml/min
 Mass of adsorbent = 6.66 g
 Initial concentration of 3-MT = 410 ppmw
 Initial concentration of Toluene = 1.09 %

Table B22 Breakthrough curve for the adsorptive removal of 3-MT and Toluene on NaX zeolite with pre-adsorbed water

Time (min)	Cumulative effluent volume (ml/g-zeolite)	C(t) of Toluene (%)	C(t) of 3-MT (%)	C(t)/C ₀ of Toluene	C(t)/C ₀ of 3-MT
2.046	1.555	0.000	0.000	0.000	0.000
4.296	3.264	0.000	0.000	0.000	0.000
6.546	4.974	0.006	0.000	0.006	0.000
8.796	6.684	0.013	0.000	0.012	0.000
11.046	8.394	0.089	0.000	0.083	0.000
13.296	10.103	0.268	0.006	0.249	0.162
15.546	11.813	0.482	0.009	0.448	0.265
17.796	13.523	0.670	0.013	0.623	0.369
20.046	15.233	0.818	0.016	0.761	0.457
22.296	16.942	0.917	0.018	0.853	0.531
24.546	18.652	0.985	0.020	0.916	0.590
26.796	20.362	1.035	0.022	0.963	0.649
29.046	22.071	1.051	0.024	0.978	0.693
31.296	23.781	1.069	0.025	0.995	0.723
33.546	25.491	1.073	0.026	0.998	0.752
35.796	27.201	1.077	0.027	1.002	0.782
38.046	28.910	1.070	0.027	0.996	0.796
40.296	30.620	1.084	0.029	1.009	0.840
42.546	32.330	1.085	0.029	1.009	0.855
44.796	34.040	1.084	0.030	1.009	0.870
47.046	35.749	1.079	0.030	1.004	0.885
49.296	37.459	1.073	0.031	0.998	0.899
51.546	39.169	1.077	0.031	1.002	0.914
53.796	40.878	1.081	0.032	1.006	0.929
56.046	42.588	1.071	0.032	0.996	0.929
58.296	44.298	1.083	0.032	1.008	0.944
60.546	46.008	1.074	0.032	0.999	0.944
62.796	47.717	1.070	0.032	0.996	0.944
65.046	49.427	1.073	0.032	0.998	0.944
67.296	51.137	1.077	0.033	1.002	0.973

Note: Flow rate = 5 ml/min
 Mass of adsorbent = 6.24 g
 Initial concentration of 3-MT = 340 ppmw
 Initial concentration of Toluene = 1.107 %

Table B23 Breakthrough curve for the adsorptive removal of 3-MT and Toluene on NiX zeolite with pre-adsorbed water

Time (min)	Cumulative effluent volume (ml/g-zeolite)	C(t) of Toluene (%)	C(t) of 3-MT (%)	C(t)/C ₀ of Toluene	C(t)/C ₀ of 3-MT
2.046	1.545	0.033	0.000	0.030	0.000
4.296	3.245	0.221	0.008	0.199	0.243
6.546	4.944	0.490	0.015	0.441	0.455
8.796	6.644	0.685	0.019	0.617	0.577
11.046	8.343	0.864	0.023	0.778	0.698
13.296	10.042	0.992	0.025	0.893	0.759
15.546	11.742	1.057	0.027	0.952	0.819
17.796	13.441	1.087	0.028	0.979	0.850
20.046	15.140	1.104	0.029	0.994	0.880
22.296	16.840	1.106	0.030	0.996	0.911
24.546	18.039	1.105	0.031	0.995	0.941
26.796	20.239	1.110	0.031	1.000	0.941
29.046	21.938	1.112	0.032	1.002	0.971
31.296	23.637	1.107	0.032	0.997	0.971
33.546	25.337	1.107	0.032	0.997	0.971
35.796	27.036	1.113	0.033	1.002	1.002
38.046	28.736	1.112	0.033	1.002	1.002
40.296	30.435	1.108	0.033	0.998	1.002
42.546	32.134	1.111	0.033	1.001	1.002
44.796	33.834	1.114	0.033	1.003	1.002
47.046	35.533	1.113	0.033	1.002	1.002
49.296	37.233	1.110	0.033	1.000	1.002
51.546	38.932	1.114	0.033	1.003	1.002
53.796	40.631	1.116	0.033	1.005	1.002
56.046	42.331	1.110	0.033	1.000	1.002
58.296	44.030	1.109	0.033	0.999	1.002
60.546	45.730	1.115	0.033	1.004	1.002
62.796	47.429	1.057	0.031	0.952	0.941
65.046	49.128	1.108	0.033	0.998	1.002
67.296	50.828	1.107	0.033	0.997	1.002

Note: Flow rate = 5 ml/min
 Mass of adsorbent = 6.62 g
 Initial concentration of 3-MT = 330 ppmw
 Initial concentration of Toluene = 1.111 %

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Academic Awards:

1. Second prize

- From the Vietnam Fund for Supporting Technological Creativity (VIFOTECH), 2005.
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2. Consolation prize

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