CHAPTER 4

MODELLING AND MODEL DISCRIMINATION

As discussed in the Chapter 3, the new models for catalytic reforming processes are therefore developed by taking into consideration the limits of all previous models. In addition, the parameters are also estimated covering all previous operating conditions. The reactor used in the new models is a fixed-bed reactor. The catalyst used   experiment is the commercial reforming catalyst, contain-ing 0.296 wt.%Pt, 0.311 wt.%Re and 0.95 wt. %Cl on a Al_2O_3 support. The BET surface area amounted to 197 m^2/g and the fraction of exposed metal atoms to 0.69. The diameters of catalyst particles are between 0.4 and 1.0 mm.

Assumptions

In the development, the following assumptions are made :

(1) A one-dimensional plug flow model is used to represent the catalytic fixed-bed reactor in which concentration and temperature gradients occur only in the axial direction.

(2) The catalytic fixed-bed reactor is operated at a steady-state flow condition.

(3) The heat flux by molecular diffusion, heat conduction and heat radiation are negligible.

(4) Pressure drop through the reactor is negligible.

(5) Since in the plant, the hydrogen partial pressure is always kept at a high value, the catalyst deactivation is therefore assumed to be neglected.

In the new models, the development of a mathematical model of the catalytic reforming we adopt and approached in which

(1) The feeds are C_6 or C_7 hydrocarbons and their mixture. The reaction network for the new models are shown in Figure 4-1 (for model 1 and 2), Figure 4-2 (for model 3).
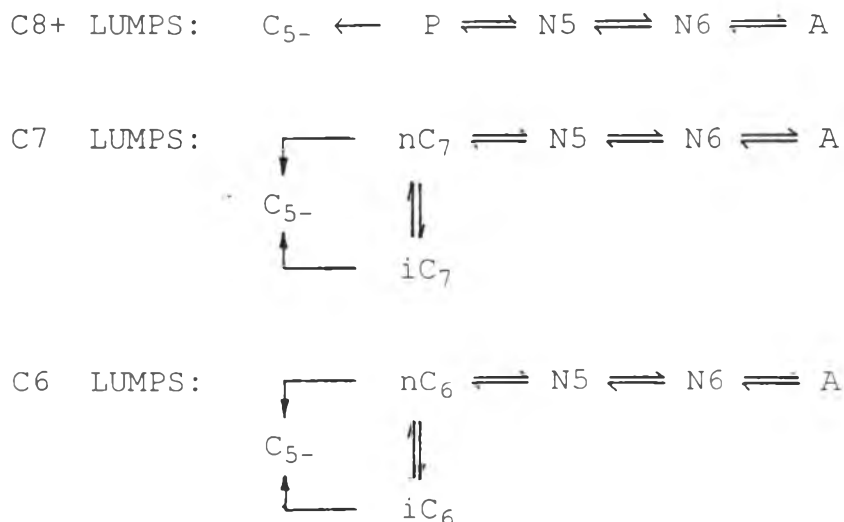
C8+ LUMPS: $C_{5-} \longleftarrow P \rightleftharpoons N5 \rightleftharpoons N6 \rightleftharpoons A$

C7 LUMPS:

$nC_7 \rightleftharpoons N5 \rightleftharpoons N6 \rightleftharpoons A$

C_{5-}

iC_7

C6 LUMPS:

$nC_6 \rightleftharpoons N5 \rightleftharpoons N6 \rightleftharpoons A$

C_{5-}

iC_6

Figure 4-1 The reaction network of the model 1 and 2

C8+ LUMPS: C_{5-} ⟵ P ⇌ N5 ⇌ N6 ⇌ A

C7 LUMPS: C_{5-} ⟵ P ⇌ N5 ⇌ N6 ⇌ A

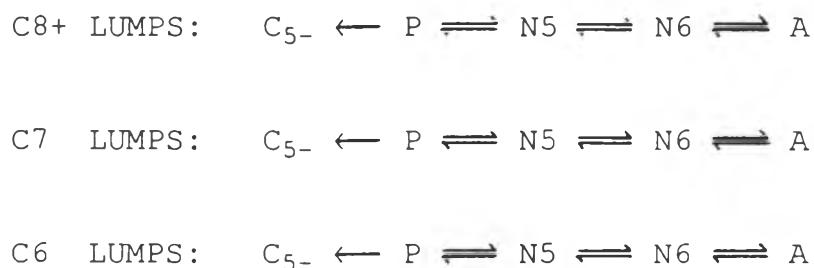C6 LUMPS: C_{5-} ⟵ P ⇌ N5 ⇌ N6 ⇌ A

Figure 4-2   The reaction network of the model 3

(2)   The equilibrium reactions of C_6 and C_7 hydro-
carbons such as benzene and toluene are negligible.

(3)   The rate equations for C_6 hydrocarbons are
obtained from Marin et al.(1982).   The main reactions are
isomerization, ring closure, ring expansion, dehydrogena-
tion of methylcyclopentane and hydrocracking.   The C_6
hydrocarbons are n-hexane, 2-methylpentane(2MP), 3-methyl-
pentane (3MP) , 2,2-dimethylbutane (22DMB) , 2,3-dimethyl-
butane(23DMB), methylcyclopentane(MCP) and benzene(Bz).

(4)   The rate equations of C_7 hydrocarbons are
obtained from Van Trimpont et al.(1986) for isomerization,
hydrocracking, ring closure, ring expansion. The C_7 hydro-
carbons are n-heptane, single-branched isoheptane(SBP$_7$),
multi-branched isoheptane (MBP$_7$), five-ring napthenes with
seven carbon atoms (5N$_7$) , methylcyclohexane (MCH) and
toluene(Tol).

(5)   The rate equation of dehydrogenation of MCH
for model 2 is obtained from Jothimurugesan et al.(1985).

The first simulation with C_6 hydrocarbons is to be
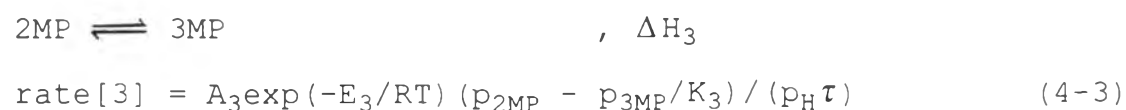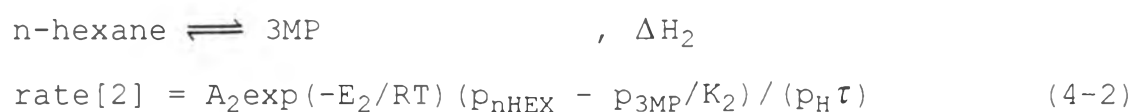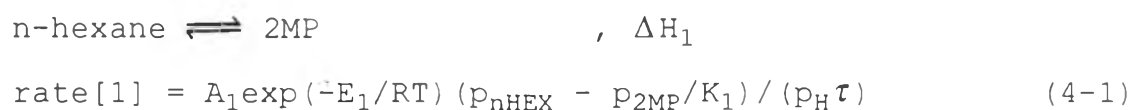compared with experimental data from Shum et al.(1985) and

Parera et al.(1986). The second simulation is C_7 hydrocarbons which to be compared with experimental data from Jothimurugesan et al. (1985), Shum et al.(1985), Van Trimpont et al. (1986), and Shantanu et al. (1988). An attempt to simulate the catalytic fixed-bed reactor for benzene and toluene from a narrow boiling mixture of C_6 and C_7 hydrocarbon is to be made and simulated results are compared with experiments of Javier et al. (1988) and Shantanu et al.(1988) by using Platinum-Rhenium Catalyst.
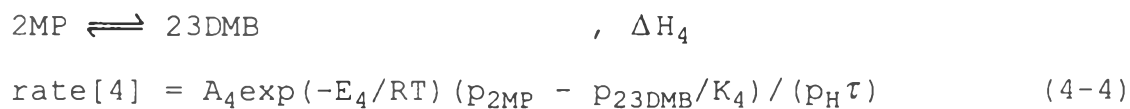
Reactor Model

Marin et al.(1982) have reported rate equations of the C_6 hydrocarbons using the Hougen-Watson rate equations. The feedstocks are n-hexane.

The rate equations for isomerization, ring closure , ring expansion, and hydrocracking can be written as:

isomerization

n-hexane $\rightleftharpoons$ 2MP , ΔH_1

$$rate[1] = A_1 \exp(-E_1/RT)(p_{nHEX} - p_{2MP}/K_1)/(p_H \tau) \tag{4-1}$$

n-hexane $\rightleftharpoons$ 3MP , ΔH_2

$$rate[2] = A_2 \exp(-E_2/RT)(p_{nHEX} - p_{3MP}/K_2)/(p_H \tau) \tag{4-2}$$

2MP $\rightleftharpoons$ 3MP , ΔH_3

$$rate[3] = A_3 \exp(-E_3/RT)(p_{2MP} - p_{3MP}/K_3)/(p_H \tau) \tag{4-3}$$

$2MP \rightleftharpoons 23DMB \qquad\qquad , \Delta H_4$

$$rate[4] = A_4 \exp(-E_4/RT)(p_{2MP} - p_{23DMB}/K_4)/(p_H \tau) \qquad (4-4)$$

$23DMB \rightleftharpoons 22DMB \qquad\qquad , \Delta H_5$

$$rate[5] = A_5 \exp(-E_5/RT)(p_{23DMB} - p_{22DMB}/K_5)/(p_H \tau) \qquad (4-5)$$

ring closure

$n\text{-hexane} \rightleftharpoons MCP + H_2 \qquad\qquad , \Delta H_6$

$$rate[6] = A_6 \exp(-E_6/RT)(p_{nHEX} - p_{MCP}p_H/K_6)/(p_H \tau) \qquad (4-6)$$

ring expansion

$MCP \rightleftharpoons benzene + 3H_2 \qquad\qquad , \Delta H_7$

$$rate[7] = A_7 \exp(-E_7/RT)(p_{MCP} - p_{Bz}p_H^3/K_7)/(p_H \tau) \qquad (4-7)$$

hydrocracking for model 1 and 2

$2MP + H_2 \longrightarrow 2C_5^- \qquad\qquad\cdot\qquad , \Delta H_8$

$$rate[8] = A_8 \exp(-E_8/RT)\cdot p_{2MP}/\tau \qquad (4-8a)$$

$3MP + H_2 \longrightarrow 2C_5^- \qquad\qquad , \Delta H_9$

$$rate[9] = A_9 \exp(-E_9/RT)\cdot p_{3MP}/\tau \qquad (4-9)$$

$23DMB + H_2 \longrightarrow 2C_5^- \qquad\qquad , \Delta H_{10}$

$$rate[10] = A_{10} \exp(-E_{10}/RT)\cdot p_{23DMB}/\tau \qquad (4-10)$$

hydrocracking for model 3

n-hexane + $H_2 \longrightarrow 2C_5^-$, ΔH_8

rate[8] = $A_8 \exp(-E_8/RT) \cdot p_{2MP}/\tau$ (4-8b)

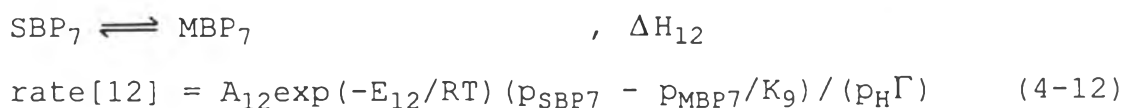A_1 to A_{10} and E_1 to E_{10} are Arrhenius constants and activation energies, respectively. p_{nHEX}, p_{2MP}, p_{3MP}, p_{22DMB}, p_{23DMB}, p_{MCP}, p_{Bz}, p_H and K_1 to K_7 are the partial pressures of n-hexane, 2-methyl-pentane, 3-methylpentane, 2,2-dimethylbutane, 2,3-dimethybutane, methylcyclopentane, benzene , hydrogen and equilibrium constant of each reaction, respectively. τ is adsorption constant.

Van Trimpont et al. (1986) have reported rate equations of C_7 hydrocarbons on commercial Pt-Re/Al_2O_3 catalyst (the rate equations of the Hougen-Watson type are used in this model). The main reforming reactions are isomerization, ring closure, ring expansion, hydrocracking and dehydrogenation of methylcyclohexane. The feedstocks are n-heptane, 2,4-dimethylpentane, methylcyclohexane and toluene.

The rate equations can be written as

Isomerization

n-heptane $\rightleftharpoons$ SBP$_7$, ΔH_{11}

rate[11] = $A_{11} \exp(-E_{11}/RT)(p_{nHEP} - p_{SBP7}/K_8)/(p_H \Gamma)$ (4-11)

SBP$_7$ $\rightleftharpoons$ MBP$_7$, ΔH_{12}

rate[12] = $A_{12} \exp(-E_{12}/RT)(p_{SBP7} - p_{MBP7}/K_9)/(p_H \Gamma)$ (4-12)

ring closure

$$n\text{-heptane} \rightleftharpoons 5N_7 + H_2 \qquad\qquad , \; \Delta H_{13}$$

$$\text{rate[13]} = A_{13}\exp(-E_{13}/RT)(p_{nHEP} - p_{5N7}p_H/K_{10})/(p_H\Gamma) \qquad (4\text{-}13)$$

ring expansion

$$5N_7 \rightleftharpoons MCH \qquad\qquad , \; \Delta H_{14}$$

$$\text{rate[14]} = A_{14}\exp(-E_{14}/RT)(p_{5N7} - p_{MCH}/K_{11})/(p_H\Gamma) \qquad (4\text{-}14)$$

dehydrogenation of methylcyclohexane for model 1,3

$$MCH \rightleftharpoons Tol + 3H_2 \qquad\qquad , \; \Delta H_{15}$$

$$\text{rate[15]} = A_{15}\exp(-E_{15}/RT)(p_{MCH} - p_{Tol}p_H^3/K_{12})/\theta \qquad (4\text{-}15a)$$

dehydrogenation of methylcyclohexane for model 2

$$MCH \rightleftharpoons Tol + 3H_2 \qquad\qquad , \; \Delta H_{15}$$
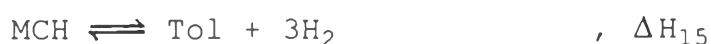
$$\text{rate[15]} = 1366\exp(-6200/T_{abs})(p_{MCH} - p_{Tol}p_H^3/K_{12})/\theta \qquad (4\text{-}15b)$$

hydrocracking

$$SBP_7 + H_2 \longrightarrow 2C_6^- \qquad\qquad , \; \Delta H_{16}$$

$$\text{rate[16]} = A_{16}\exp(-E_{16}/RT)\cdot p_{SBP7}/(p_H\Gamma) \qquad (4\text{-}16a)$$

$$MBP_7 + H_2 \longrightarrow 2C_6^- \qquad\qquad , \; \Delta H_{17}$$

$$\text{rate[17]} = A_{17}\exp(-E_{17}/RT)\cdot p_{MBP7}/(p_H\Gamma) \qquad (4\text{-}17)$$

hydrocracking for model 3

n-heptane + $H_2 \longrightarrow 2C_6^-$, ΔH_{16}
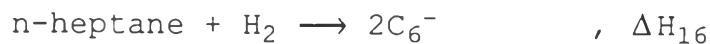
rate[16] = $A_{16}\exp(-E_{16}/RT) \cdot p_{SBP7}/(p_H\Gamma)$ (4-16b)

p_{nHEP}, p_{SBP7}, p_{MBP7}, p_{5N7}, p_{MCH}, p_{Tol} and p_H are the partial pressures of n-heptane , single-branched iso-heptane , multi-branched isoheptane, five-ring napthenes with seven atoms, methylcyclohexane, toluene and hydrogen, respectively. Γ and θ are the adsorption constants for acid and metal adsorption terms.

Model Development

Material balance is

$$\frac{dx_j}{d(W / F_{HC})} = R_j \qquad (4-18)$$

Energy Balance is

$$\left(\sum_j \frac{F_j Cp_j}{F_{HC}}\right) \frac{dT}{d(W / F_{HC})} = \sum_i (-\Delta H_i) r_i \qquad (4-19)$$

where R_j is net rate of multi-reaction of component j

r_i is reaction rate of component i

F_j is molar flow rate of component j

F_{j0} is molar flow rate of component j at initial condition

W is weight of catalyst

T   is temperature

X_j is fraction conversion of component j

Cp_j is heat capacity of component j

ΔH_i is heat of reaction of reaction i

For example, the global rate of reactions of model 1 for different component of C_6 and C_7 hydrocarbons are given as follows:

$\underline{C_6\ hydrocarbons}$

$$F[1] \quad = \frac{d\ X_{nHEX}}{d(W\ /\ F_{HC})} = -rate[1]-rate[2]-rate[6] \qquad (4\text{-}20)$$

$$F[2] \quad = \frac{d\ X_{2MP}}{d(W\ /\ F_{HC})} = rate[1]-rate[3]-rate[4]-rate[8] \quad (4\text{-}21)$$

$$F[3] \quad = \frac{d\ X_{3MP}}{d(W\ /\ F_{HC})} = rate[2]+rate[3]-rate[7] \qquad (4\text{-}22)$$

$$F[4] \quad = \frac{d\ X_{22DMB}}{d(W\ /\ F_{HC})} = rate[5]-rate[10] \qquad (4\text{-}23)$$

$$F[5] \quad = \frac{d\ X_{23DMB}}{d(W\ /\ F_{HC})} = rate[4]-rate[5] \qquad (4\text{-}24)$$

$$F[6] \quad = \frac{d\ X_{MCP}}{d(W\ /\ F_{HC})} = rate[6]-rate[7] \qquad (4\text{-}25)$$

$$F[7] \quad = \frac{d\ X_{BZ}}{d(W\ /\ F_{HC})} = rate[7] \qquad (4\text{-}26)$$

$$F[8] = \frac{d\ X_H}{d(W\ /\ F_{HC})} = rate[6]+3.rate[7]-rate[8]-rate[9]-rate[10]$$

$$(4\text{-}27)$$

$$F[9] = \frac{d\,X_{C5}}{d(W\,/\,F_{HC})} = (rate[8]+rate[9]+rate[10]).2 \qquad (4\text{-}28)$$

C_7 hydrocarbons

$$F[10] = \frac{d\,X_{nHEP}}{d(W\,/\,F_{HC})} = -rate[11]-rate[13] \qquad (4\text{-}29)$$

$$F[11] = \frac{d\,X_{Tol}}{d(W\,/\,F_{HC})} = rate[15] \qquad (4\text{-}30)$$

$$F[12] = \frac{d\,X_{MCH}}{d(W\,/\,F_{HC})} = rate[14]-rate[15] \qquad (4\text{-}31)$$

$$F[13] = \frac{d\,X_{5N7}}{d(W\,/\,F_{HC})} = rate[13]-rate[14] \qquad (4\text{-}32)$$

$$F[14] = \frac{d\,X_{SBP7}}{d(W\,/\,F_{HC})} = rate[11]-rate[12]-rate[16] \qquad (4\text{-}33)$$

$$F[15] = \frac{d\,X_{MBP7}}{d(W\,/\,F_{HC})} = rate[12]-rate[17] \qquad (4\text{-}34)$$

$$F[16] = \frac{d\,X_{H}}{d(W\,/\,F_{HC})} = rate[13]+3.rate[15]-rate[16]-rate[17]$$

$$(4\text{-}35)$$

$$F[17] = \frac{d\,X_{C6}}{d(W\,/\,F_{HC})} = (rate[16]+rate[17]).2 \qquad (4\text{-}36)$$

The material balance and energy balance equations for various components are obtained after the mole fraction of all reaction systems and the total pressure are substituted by $p_i = x_i P$ in the equation i where x_i is the mole fraction of component i. The energy balance equation can be written as

C$_6$ hydrocarbons

$$\left(\frac{dT}{d(W / F_{HC})}\right)_1 = \frac{1}{Cp_{MIX}}\left[(-\Delta H_1)rate[1] + (-\Delta H_2)rate[2] + \right.$$

$$(-\Delta H_3)rate[3] + (-\Delta H_4)rate[4] +$$

$$(-\Delta H_5)rate[5] + (-\Delta H_6)rate[6] +$$

$$(-\Delta H_7)rate[7] + (-\Delta H_8)rate[8] +$$

$$\left. (-\Delta H_9)rate[9] + (-\Delta H_{10})rate[10]\right]$$

$$(4-37)$$

C$_7$ hydrocarbons

$$\left(\frac{dT}{d(W / F_{HC})}\right)_2 = \frac{1}{Cp_{MIX}}\left[(-\Delta H_{11})rate[11] + (-\Delta H_{12})rate[12] + \right.$$

$$(-\Delta H_{13})rate[13] + (-\Delta H_{14})rate[14] +$$

$$(-\Delta H_{15})rate[15] + (-\Delta H_{16})rate[16] +$$

$$\left. (-\Delta H_{17})rate[17]\right]$$

$$(4-38)$$

where Cp_{MIX} is the heat capacity of gas mixture

$F_{HC}°$ is the total molar flow rate of hydrocarbons
at initial condition

The overall rate of temperature change along the reactor is

$$F[17] = \left(\frac{dT}{d(W / F_{HC})}\right)_{overall} = \left(\frac{dT}{d(W / F_{HC})}\right)_1 + \left(\frac{dT}{d(W / F_{HC})}\right)_2$$

$$(4-39)$$

Thus, the mathematical model can be written in a set of system equations as

C_6 hydrocarbons

$$F[N] = f(X_{nHEX}, X_{2MP}, X_{3MP}, X_{22DMB}, X_{23DMB}, X_{MCP}, X_{Bz}, X_H,$$
$$X_{C5^-}, T, P)$$

$$(4-40)$$

where $N = 1, 2, \ldots, 9$

The boundary conditions at $W/F_{HC}^\circ = 0$, X_{nHEX}, X_{2MP}, X_{3MP}, X_{22DMB}, X_{23DMB}, X_{MCP}, X_{Bz}, X_H, $X_{C5^-} = 0$, $T = T_{IN}$, where T_{IN} is the temperature at the reactor inlet.

C_7 hydrocarbons

$$F[N] = f(X_{nHEP}, X_{Tol}, X_{MCH}, X_{5N7}, X_{SBP7}, X_{MBP7}, X_H, X_{C6^-},$$
$$T, P)$$

$$(4-41)$$

where $N = 10, 11 \ldots, 17$

The boundary conditions at $W/F_{HC}^\circ = 0$, X_{nHEP}, X_{Tol}, X_{MCH}, X_{5N7}, X_{SBP7}, X_{MBP7}, X_H, $X_{C6^-} = 0$, $T = T_{IN}$.

From the models of C_6 hydrocarbons (Equation 4-20 to 4-28) and C_7 hydrocarbons (Equation 4-29 to 4-36), we can solve the parameters for all models. The best model can predict the process behavior and give the response which

close to the experimental data(see input data in Appendix E). The model can be predicted in the temperature range 325-505 °C, under pressure 1-15 bar and feedstock is C_6 or C_7 hydrocarbons or their mixture.

The values of Arrhenius constants(A) and activation energies (E) from parameter estimation by MATLAB (see parameter estimation in Appendix F) are shown in Table 4-1 (for model 1 and 2), Table 4-2 (for model 1), Table 4-3 (for model 2), Table 4-4 and Table 4-5 (for model 3).

Table 4-1 Arrhenius constants, activation energies and adsorption constants for C_6 hydrocarbons (model 1 and 2)

Reaction	A_i (kmole/kg cat.h)	E_i (kJ/mole)
Isomerization	$A_1 = 7.34 \times 10^{10}$	134.8
	$A_2 = 7.34 \times 10^{10}$	134.8
	$A_3 = 5.22 \times 10^{08}$	114.9
	$A_4 = 1.46 \times 10^{10}$	134.9
	$A_5 = 6.13 \times 10^{08}$	114.9
Ring closure	$A_6 = 4.45 \times 10^{18}$	258.7
Ring expansion	$A_7 = 1.04 \times 10^{11}$	120.7
Hydrocracking	$A_8 = 1.42 \times 10^{09}$	132.1
	$A_9 = 1.42 \times 10^{09}$	132.1
	$A_{10} = 1.73 \times 10^{09}$	132.1

Adsorption term :

$$\tau = (1+K_{HEX}+ (p_{nHEX}+p_{2MP}+p_{3MP}+p_{22DMB}+p_{23DMB})/p_H + K_{MCP}\, p_{MCP}/p_H)^2$$

$K_{HEX} = 8.389$, $K_{MCP} = 195.9$

Table 4-2 Arrhenius constants, activation energies and adsorption constants for C_7 hydrocarbons (model 1)

Reaction	A_i (kmole/kg cat.h)	E_i (kJ/mole)
Isomerization	$A_{11} = 3.82 \times 10^{14}$	192.5
	$A_{12} = 1.52 \times 10^{14}$	192.5
Ring closure	$A_{13} = 1.02 \times 10^{31}$	429.1
Ring expansion	$A_{14} = 1.84 \times 10^{24}$	319.1
Dehydrogenation of		
methylcyclohexane	$A_{15} = 8.57 \times 10^{10a}$	145.1
Hydrocracking	$A_{16} = 1.60 \times 10^{17}$	231.4
	$A_{17} = 1.60 \times 10^{17}$	231.4

Adsorption term for the acid function:

$$\Gamma = (p_H + KC_6^- \, pC_6^- + K_{P7} \, p_{P7} + K_{Tol} \, p_{Tol} \, p_H)/p_H$$

$$K_{C6-} = 90.1 \; , \; K_{P7} = 9.0 \; , \; K_{Tol} = 7.5 \text{ bar}^{-1}$$

Adsorption term for the metal function:

$$\theta = 1 + K_{nHEP} \, p_{nHEP} + K_{MCH} \, p_{MCH} + K_{Tol} \, p_{Tol}$$

$$K_{nHEP} = 1.84 \text{ bar}^{-1}, \; K_{MCH} = 1.98 \text{ bar}^{-1}, \; K_{Tol} = 10.4$$

$$\text{bar}^{-1}$$

[a] Units in kmole/(kg cat.h.bar)

Table 4-3 Arrhenius constants, activation energies and adsorption constants for C_7 hydrocarbons (model 2)

Reaction	A_i (kmole/kg cat.h)	E_i (kJ/mole)
Isomerization	$A_{11} = 4.92 \times 10^{14}$	197.7
	$A_{12} = 1.65 \times 10^{14}$	197.7
Ring closure	$A_{13} = 6.41 \times 10^{30}$	437.4
Ring expansion	$A_{14} = 1.08 \times 10^{25}$	326.8
Dehydrogenation of methylcyclohexane	$A_{15} = 2.10 \times 10^{11}$[a]	152.4
Hydrocracking	$A_{16} = 3.44 \times 10^{17}$	248.5
	$A_{17} = 3.44 \times 10^{17}$	248.5

Adsorption term for the acid function:

$$\Gamma = (p_H + K_{C6-}\, p_{C6-} + K_{P7}\, p_{P7} + K_{Tol}\, p_{Tol}\, p_H)/p_H$$

$$K_{C6-} = 90.1 \ , \ K_{P7} = 9.0 \ , \ K_{Tol} = 7.5 \text{ bar}^{-1}$$

Adsorption term for the metal function:

$$\theta = 1 + K_{Tol}\, p_{Tol}$$

$$K_{Tol} = 0.0633\exp(1600/T_{abs})$$

[a] Units in kmole/(kg cat.h.bar)

Table 4-4 Arrhenius constants, activation energies and adsorption constants for C_6 hydrocarbons (model 3)

Reaction	A_i (kmole/kg cat.h)	E_i (kJ/mole)
Ring closure	$A_1 = 4.52 \times 10^{17}$	254.6
Ring expansion	$A_2 = 9.49 \times 10^{10}$	137.3
Hydrocracking	$A_3 = 1.07 \times 10^{09}$	147.3

Adsorption term :

$$\tau = (1 + K_{HEX} + (p_{nHEX} + p_{2MP} + p_{3MP} + p_{22DMB} + p_{23DMB})/p_H + K_{MCP}\, p_{MCP}/p_H)^2$$

$K_{HEX} = 8.389$, $K_{MCP} = 195.9$

Table 4-5 Arrhenius constants, activation energies and adsorption constants for C_7 hydrocarbons

Reaction	A_i (kmole/kg cat.h)	E_i (kJ/mole)
Ring closure	$A_4 = 2.77 \times 10^{31}$	450.4
Ring expansion	$A_5 = 1.15 \times 10^{24}$	331.6
Dehydrogenation of methylcyclohexane	$A_6 = 2.48 \times 10^{11a}$	147.6
Hydrocracking	$A_7 = 1.22 \times 10^{17}$	241.0

Adsorption term for the acid function:

$$\Gamma = (p_H + K_{C_6^-}\, p_{C_6^-} + K_{P7}\, p_{P7} + K_{Tol}\, p_{Tol}\, p_H)/p_H$$

$K_{C6-} = 90.1$, $K_{P7} = 9.0$, $K_{Tol} = 7.5$ bar^{-1}

Adsorption term for the metal function:

$$\theta = 1 + K_{nHEP}\, p_{nHEP} + K_{MCH}\, p_{MCH} + K_{Tol}\, p_{Tol}$$

$K_{nHEP} = 1.84$ bar^{-1}, $K_{MCH} = 1.98$ bar^{-1}, $K_{Tol} = 10.4$ bar^{-1}

Comparison of Model Fitting

The errors between model fitting and experimental data for the new models are shown in Table 4-6.

Table 4-6 Comparison of Model Fitting

		Error = $\sum_i (Y_i - \overline{Y_i})^2$		
CASE	COMPONENT	MODEL 1	MODEL 2	MODEL 3
1	iC_6	0.50	0.50	-
	C_{5-}	0.33	0.33	0.90
	Bz	0.36	0.36	1.20
2	iC_6	0.13	0.13	-
	C_{5-}	0.64	0.64	1.10
	Bz	0.37	0.37	1.40
3	iC_6	0.10	0.10	-
	C_{5-}	1.17	1.17	1.90
	Bz	0.09	0.09	0.54
4	iC_7	0.68	0.86	-
	C_{6-}	0.86	1.02	1.10
	Toluene	0.04	0.77	0.97
5	iC_7	1.07	2.65	-
	5N7	0.03	0.77	-
	C_{6-}	1.03	2.38	2.55
	Toluene	0.74	1.42	1.79
6	iC_7	0.82	2.38	-
	C_{6-}	0.17	1.61	1.73
	Toluene	0.86	1.17	1.33
7	Toluene	0.06	0.03	0.12
8	Toluene	0.07	0.07	0.26
9	Toluene	0.26	0.19	0.44
10	Toluene	0.41	0.43	0.69
11	Toluene	0.03	0.10	0.15
12	Toluene	0.28	0.55	0.66

Table 4-6 Comparison of Model Fitting(continued)

| CASE | COMPONENT | Error = $\sum_{i}(Y_i - \overline{Y}_i)^2$ | | |
		MODEL 1	MODEL 2	MODEL 3
13	Toluene	0.01	0.12	0.38
14	Toluene	0.47	0.53	0.91
15	Toluene	0.03	0.31	0.35
16	Toluene	0.01	0.35	0.63
17	Toluene	0.07	0.46	0.99
18	Toluene	0.03	0.66	0.72
19	Toluene	0.03	0.66	0.64
20	Bz	0.03	0.03	0.37
	Toluene	0.33	0.62	0.88
21	Bz	0.05	0.05	0.42
	Toluene	0.09	0.75	0.76

From Table 4-6, the data were most satisfactorily correlated by model 1 while the model 2 is suitable for pure methylcyclohexane feedstock only and the errors of model 3 are higher than the errors of model 1 and model 2. Therefore, the model 1 is the most appropriate to use for this study.