A Kinetic Hydrocracking Model for Aromatic Feed

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Hydrocracking feedstocks contain a wide variation in the concentration of various compunds types, i. e. paraffins, mono- and poly-cyclo paraffins and mono- and cycloaromatics. Typical hydrocracking feedstocks, like vacuum gasoil (VGO) and coker gasoil (CGO) contain large fractions of mono- and polyaromatics (approx. 50 %). On a bifunctional catalyst, i. e. hydrogenation and cracking sites, the aromatic rings is subsequent hydrogenated and cracked. The hydrocracking kinetic model developed for aromatic feed on bifunctional catalyst is based on the individual steps of both hydrogenation and cracking. Under steady state process conditions the rate equation of both reactions can be reduced to first order kinetics in respect to the reactant organic compounds. The developed kinetic model predicts the yield of a hydrocracking aromatic kinetic scheme containing 15 pseudo-components as function of residence time.

Ausgangsstoffe für den Hydrocracker enthalten eine Reihe von Verbindungstypen (Paraffine, Mono- und Polycyclo-Paraffine, Mono- und Cycloaromaten) in unterschiedlicher Konzentration. Typische Produkte wie Vakuumgasöl (VGO) und Kokergasöl (CGO) enthalten einen hohen Anteil an Mono- und Polyaromaten (ca. 50 %). Ein bifunktionaler Katalysator mit entsprechenden Aktivzentren bewirkt Hydrierung und Cracken des Aromatenrings nacheinander. Das kinetische Modell für Hydrocrackung eines aromatischen Ausgangsstoffes auf einen bifunktionalen Katalysator beruht auf die beiden genannten Reaktionsschritte. Unter Gleichgewichtsbedingungen handelts es sich in beiden Fällen um eine Reaktion 1. Ordnung. Das kinetische Modell ermöglicht die Vorhersage der Ausbeute eines Schemas mit 15 Pseudokomponenten als Funktion der Verweilzeit.

Introduction

Hydrocracking is one of the most versitale processing steps available to modern refineries. The flexibility of hydrocracking is emphasized by the number of treated feedstocks and the variety of obtained products, as shown in *table I*. The hydro carbon feed to be cracked represents a spectrum of pure hydrocarbons of molecular weights ranging from 100–500 and of varying proportions of paraffins, aromatics and naphthenes. This variation in compound type distribution has a significant influence on the design and operation of a hydrocracker.

Table I: Typical hydrocracking feedstocks and products

Feed	Products
Straight Run Gas Oils	LPG
Vacuum Gas Oils	Motor Gasolines
Fluid Catalytic Cracking Oils	Reformer Feeds
Coker Gas Oil	Aviation Turbine Fuels
Thermally Cracked Stocks	Diesel Fuels
Solvent Deasphalted Residual Oils	Heating Oils
	Solvent and thinners
Straight Run Naphtha	Lube Oils
Cracked Naphtha	Petrochemical feedstocks

Since 1960 a number of kinetic models to predict hydrocracker yields are developed, based on boiling distributions [1, 2, 3] or the definition of pseudo components of feed and product [4, 5, 6]. Except the yield of the various products, refiners are interested in the obtained quality. The model presented is a first step to come to a quality prediction of hydrocracking products next to the yield. The model components are to be classified to the quality criteria of products, like the octane number of gasoline, the cetane number of diesel and the smoke point of jet fuel.

The hydrocracking catalyst is a careful combination of hydrogenation and the cracking components, as shown in *table II*. The cracking component, for example amorphous silica-alumina or zeolite provides the acidic function. The hydrogenation components are noble metals (Pt, Pd) or non noble metals (Ni, Mo, W). The developed model is based on individual steps of both hydrogenation and cracking on a bifunctional catalyst.

Table II: Bifunctional hydrocracking catalyst

Hydrogenation function		Acidic function	
	↓ Ni/Mo	Al_2O_3 ↓	
Increasing	↓ Ni/W	Al_2O_3/halogen ↓	Increasing
hydrogenation	↓ Pt/Pd		
power	↓	SiO_2/Al_2O_3 ↓	acidity
		Zeolite ↓	

The developed kinetic model

The hydrocracking reaction scheme of aromatics as shown in *figure 1.* is proposed by *Laux et al.* [5]. The horizontal reactions in the scheme are the cracking reactions, while the vertical reactions are the hydrogenation reactions. Calculations of the thermo-dynamic fundamental equation confirmed that only the reaction of mono-aromatics to naphthenes is reversible under hydrocracking process conditions (P > 15 MPa, T 350–450 °C) [5]. *Qader et al.* [1, 7] concluded on the apparent activation energy, that for pressures higher than 12 MPa the surface reaction is the rate controlling.

The overall reaction rate for hydrogenation and cracking can be represented by:

Hydrogenation: $A_iN_j + \nu H_2 \leftrightarrows A_{(i-\nu/2)}\,N_{(j+\nu/2)}$ (ν = 0,2,4,6 etc.)
Cracking: $A_iN_j \rightarrow A_iN_{(j-1)} + P$

The subsequent hydrocracking reactions taking place on a bifunctional catalyst is illustrated in *figure 2*.

The kinetic model is based on the following assumptions:

- Uniform adsorptive hydrogenation and cracking sites.
- Unimolecular layer of adsorbate on the catalyst surface.
- Existance of an adsorption and desorption quasi equilibrium of the various compounds on the catalyst surface.
- Surface reaction rate determining [7].
- All surface reactions are irreversible [5].
- Isothermal over the reactor

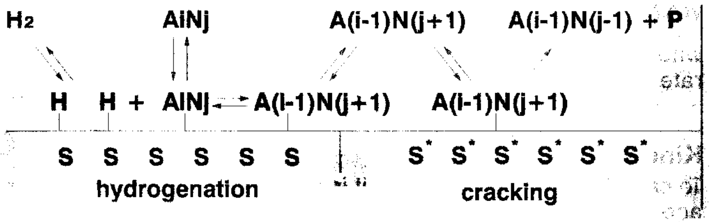

Figure 1: The hydrocracker reaction scheme of aromatics

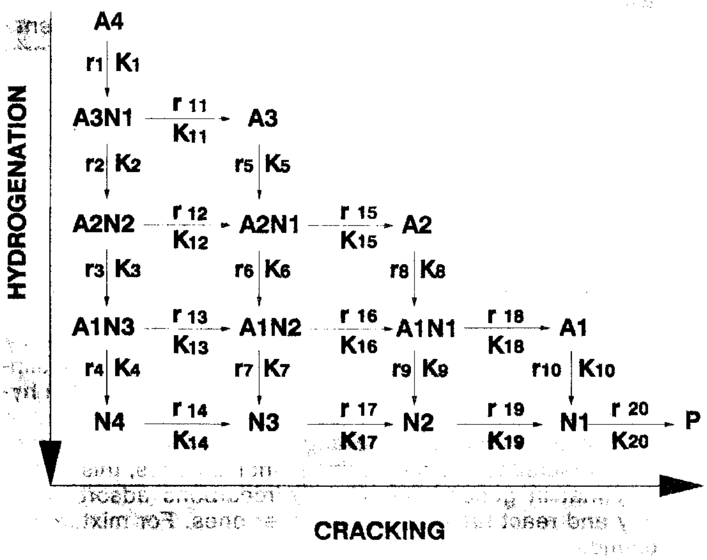

Figure 2: Visualization hydrocracking surface reaction

Hydrogenation individual steps

Rates of bimolecular reactions controlled by chemical reactions taking place at the catalyst surface are known to occur due to the interaction of two reactant molecules adsorbed on neighboring active sites according to the mechanism by *Langmuir* and *Hinselwood.*

The individual steps of hydrogenation are:

$A_iN_j + S \leftrightarrows A_iN_j\text{-}S$ (adsorption, $K_A=k_a/k_{-a}$)
$H_2 + 2\,S \leftrightarrows 2\,H\text{-}S$ (adsorption, $K_H=k_h/k_{-h}$)
$A_iN_j\text{-}S + 4\,H\text{-}S \rightarrow A_{i-1}N_{j+1}\text{-}S + 4S$ (surface reaction, K_s)
$A_{i-1}N_{j+1}\text{-}S \leftrightarrows A_{j-1}N_{j+1} + S$ (desorption of product, $K_D=k_d/k_{-d}$)

If the surface reaction is rate controlling and irreversible the disappearance due to hydrogenation of the aromatic compound A_iN_j is:

$$-r(A_iN_j) = -r_s = K_s\cdot[A_iN_j\text{-}S]\cdot[H\text{-}S]^4 \qquad (1)$$

The equilibrium relations are:

$$K_A=[A_iN_j\text{-}S]/([A_iN_j]\cdot C_v) \rightarrow [A_jN_j\text{-}S] = K_A\cdot[A_iN_j]\cdot C_v \qquad (2)$$

$$K_H=[H\text{-}S]^2/([H_2]\cdot C_v^2) \rightarrow [H\text{-}S] = (K_H\cdot[H_2])^{1/2}\cdot C_v \qquad (3)$$

$$K_D=([A_{i-1}N_{j+1}]\cdot C_v)/[A_{i-1}N_{j+1}\text{-}S] \rightarrow [A_{i-1}N_{j+1}\text{-}S] = K_D^{-1}\cdot[A_{i-1}N_{j+1}]\cdot C_v \qquad (4)$$

where C_v is the surface concentration of vacant sites.

Using Eqs. 2 and 3 in 1 results in:

$$-r(A_iN_j) = K_S\cdot K_A\cdot[A_iN_j]\cdot C_v\cdot K_H^2\cdot[H_2]^2\cdot C_v^4 = K_S\cdot K_A\cdot K_H^2\cdot C_v^5\cdot[H_2]^2\cdot[A_iN_j] \qquad (5)$$

In addition, a relation for the total quantity active hydrogenation sites C_t is:

$$C_t = [S]+[H\text{-}S]+\sum_{m=1}^{m=4}\sum_{n=0}^{n=m}[A_nN_m\text{-}S] \qquad (6)$$

Using Eqs. 2 and 3 in 6 results in:

$$C_v = \frac{C_t}{1+\sqrt{K_H\cdot[H_2]}+\sum_{m=1}^{m=4}\sum_{n=0}^{n=m}K_{A,A_nN_m}\cdot[A_nN_m]} \qquad (7)$$

The rate of disappearance of A_iN_j can be written Eq. 5 using Eq. 7, as:

$$-\frac{d\,A_iN_j}{d\,t} = -t_{A_iN_j} = \frac{K_SK_A\cdot K_H^2\cdot C_t^5\cdot[H_2]^2\cdot[A_iN_j]}{\left(1+\sqrt{K_H\cdot[H_2]}+\sum_{m=1}^{m=4}\sum_{n=0}^{n=m}K_{A,A_nN_m}\cdot[A_nN_m]\right)} \qquad (8)$$

Due to the high excess of hydrogen, the concentration over the reactor can be assumed constant. Under steady state conditions the vacant site concentration can be considered constant. The rate equation (8) is reduced to a first order equation by introducing the observed rate constant ($K_{obs.}$):

$$-r(A_iN_j) = K_{h,\,obs.}\cdot[A_iN_j] \qquad (9)$$

Where,

$$K_{h,obs.} = \frac{K_SK_A\cdot K_H^2\cdot C_t^5\cdot[H_2]^2}{\left(1+\sqrt{K_H\cdot[H_2]}+\sum_{m=1}^{m=4}\sum_{n=0}^{n=m}K_{A,A_nN_m}\cdot[A_nN_m]\right)} \qquad (10)$$

$$= K_S\cdot K_A\cdot K_H^2\cdot C_v^5\cdot[H_2]^2$$

Cracking individual steps

The individual steps of cracking, as shown in *figure 2*, are:

$A_iN_j + S^* \leftrightarrows A_iN_j\text{-}S^*$ (adsorption, $K_A^* = k_a/k_{-a}$)
$A_iN_j\text{-}S^* \rightarrow A_iN_{j-1} + P + S^*$ (surface reaction, K_S^*)

Occurrence of ring opening, skeletal rearrangement, isomerization and cleavage on the acid sites of A_iN_j results in the desorption of the cracked compound and a paraffin/olefin. If the surface reaction is rate controlling and irreversible, the disappearance of the aromatic compound due to cracking is:

$$-r(A_iN_j) = -r_s = K_s^*\cdot[A_iN_j\text{-}S^*] \qquad (11)$$

The equilibrium relation is:

$$K_A^* = [A_iN_j\text{-}S^*]/([A_iN_j]\cdot C_v^*) \rightarrow [A_iN_j\text{-}S^*] = K_A^*\cdot A_iN_j]\cdot C_v^* \qquad (12)$$

where C_v^* is the surface concentration of vacant cracking sites.

Using Eqs. 11 and 12 results in:

$$-r(A_iN_j) = K_S\cdot K_A\cdot[A_iN_j]\cdot[S] = K_S^*\cdot K_A^*\cdot C_v^*\cdot[A_iN_j] \qquad (13)$$

In addition, a relation for the total active cracking sites C_v^* is:

$$C_t^* = [S^*] + \sum_{m=1}^{m=4} \sum_{n=0}^{n=m-1} [A_nN_{m-n}-S^*] \tag{14}$$

Using Eqs. 12 and 14 results in:

$$C_v^* = \frac{C_t^*}{1 + \sum_{m=1}^{m=4} \sum_{n=0}^{n=m-1} K^*_{A,A_nN_{m-n}} \cdot [A_nN_{m-n}]} \tag{15}$$

The rate of dissappearance of A_iN_j can be written from Eq. 13 using Eq. 15, as:

$$\frac{d\,A_iN_j}{d\,t} = -r_{A_iN_j}$$

$$= \frac{K_S^* \cdot K_A^* \cdot C_t^* \cdot [A_iN_j]}{1 + \sum_{m=1}^{m=4} \sum_{n=0}^{n=m-n} K^*_{A,A_nN_{m-n}} \cdot [A_nN_{m-n}]} \tag{16}$$

Under steady state conditions the vacant sites can be considered constant, by introducing the observed cracking rate constant $K_{c,\,obs}$ the cracking rate equation is reduced to first order kinetics:

$$r(A_iN_j) = K_{c,\,obs.} \cdot [A_iN_j] \tag{17}$$

Where,

$$K_{c,obs.} = \frac{K_S^* \cdot K_A^* \cdot C_t^*}{1 + \sum_{m=1}^{m=4} \sum_{n=0}^{n=m-n} K^*_{A,A_nN_{m-n}} \cdot [A_nN_{m-n}]} = K_S^* \cdot K_A^* \cdot C_v^* \tag{18}$$

The disappearance of component A_iN_j in a hydrocracker is a combination of hydrogenation and cracking of the component.

$-r(A_iN_j) = -r_h + (-r_c) = K_{h,\,obs} \cdot [A_iN_j] + K_{c.\,obs} \cdot [A_iN_j] = (K_{h,\,obs} + K_{c,\,obs}) \cdot [A_iN_j] = K_{HC,\,obs} \cdot [A_iN_j]$

The developed first order kinetics for the hydrocracking reaction was also concluded by experimental work by *Qader et al.* [1, 7] and *Hisamitsu* [8] for various feedstock types.

Rate equations

The rate equations of the 15 components of the reaction scheme are a combination of hydrogenation and cracking first order equations, respecitvely represented by r_1 to r_{10} and r_{11} to r_{20}.

$$\begin{aligned}
-r(A_4) &= r_1 \\
-r(A_3N_1) &= r_2 + r_{11} - r_1 \\
-r(A_3) &= r_5 - r_{11} \\
-r(A_2N_2) &= r_3 + r_{12} - r_2 \\
-r(A_2N_1) &= r_6 + r_{15} - r_5 - r_{12} \\
-r(A_2) &= r_8 - r_{15} \\
-r(A_1N_3) &= r_4 + r_{13} - r_3 \\
-r(A_1N_2) &= r_7 + r_{16} - r_6 - r_{13} \\
-r(A_1N_1) &= r_9 + r_{18} - r_8 - r_{16} \\
-r(A_1) &= r_{10} - r_{18} \\
-r(N_4) &= r_{14} - r_4 \\
-r(N_3) &= r_{17} - r_7 - r_{14} \\
-r(N_2) &= r_{19} - r_9 - r_{17} \\
-r(N_1) &= r_{20} - r_{10} - r_{19}
\end{aligned}$$

The rate equations are first order differential equations of the form:

$$\frac{d\gamma}{d\,x} + P\gamma = Q$$

By multiplying through with the integrating factor $e^{\int P dx}$ the solution is:

$$\gamma \cdot e^{\int P dx} = \int Q e^{\int P dx} \cdot dx + \text{constant}$$

The constant of integration is determined by the definition of the initial condition, i. e. $[A_iN_j] = [A_iN_j]_0$ at $t = 0$. The final equations expressed in molar units are to be converted to more commonly used units of weight fraction yield in respect to the feed of the reactor. The relation between the weight fraction to the molar concentration is: $[A_iN_j] = y \cdot \varrho_f/M_{w,\,Ai}N_j$. Substitution of this equation in the final concentration expressions results in a total of 15 equation of the form:

$$y(A_iN_j) = C_1 \cdot e^{K_\alpha t} + C_2 \cdot e^{K_\beta t} + \ldots + C_n \cdot e^{K_\gamma t}$$

where the constant C_1 is a mathematical relation of the ratio of rate constants, the initial weight fraction and the molar weight.

Kinetic simulations

To calculate the yield change, it is necessary to define the average molar weight, the weight fraction of the pseudo-components and the 20 rate constants of the kinetic scheme. The average molar weight of the pseudo-component is necessary to calculate relative weight change, due to the hydrogenation or cracking of the reactant molecules. In the kinetic program the molar weights of the non-alkylated molecules were used.

The composition of hydrocracker feed was determined in detail by *Yan* [9]. *Table III* illustrates the composition of fresh feed (20.4 wt% light coker gasoil, 12.4 wt% heavy gas-oil, 19.3 wt% light catalytic cracker gas-oil and 47.9 wt% heavy cracker gas-oil) and of the fractionator bottom ("unconverted"). Based on a mixture of fresh feed and recycle bottoms, as shown in *table III*, the weight fractions of the pseudo-components were estimated.

The applied Arrhenius equations, specified by the frequency factor k_0 (h^{-1}) and the activation energy (ΔE kJ/mol), in the simulation are shown in *table IV.* In the model by *Turek* [4], the hydrogenation and cracking rate constants of vacuum residue were identified. According to *Stangeland* [3] the reaction rate constant K increases as the boiling point increases, this due to the fact that in general, heavier hydrocarbons adsorb more strongly and react faster than do lighter ones. For mixtures of compounds, there is an additional effect of adsorption on relative reaction rates. *Maxwell* [10] concluded that poly aromatic structures are faster hydrogenated then mono aromatic structures. Paraffins, especially straight chain compounds, show a significant lower activity than cyclo-paraffins [11].

The yield change as function of the residence time was calculated for the pseudo components at a reactor temperature of 400 °C, as shown in *figure 3.* The decrease of residual aromatics, the aromatic pseudo-components (A_4, A_3, A_2, A_1), is continuous. The partial hydrogenated components (A_iN_j) all show a maximum, while the paraffine content is constant.

By adjusting the bed temperature of the hydrocracker the yield of the different products can be varied over a broad range [1]. In *figure 4.* and *5.* the yield change at resp. a reactor temperature of 400 and 450 °C is shown. The pseudo-components are clustered by aromatic-ring content and by the total ring content, representing respectively the hydrogenation activity (top graph) and the cracking activity (bottom graph).

At a bed temperature of 400 °C both hydrogenation and cracking activity are low. Increasing the temperature to 450 °C results in a significant enhanced hydrogenation and cracking activity are low. At elevated temperatures there is a distinct increase in paraffin content.

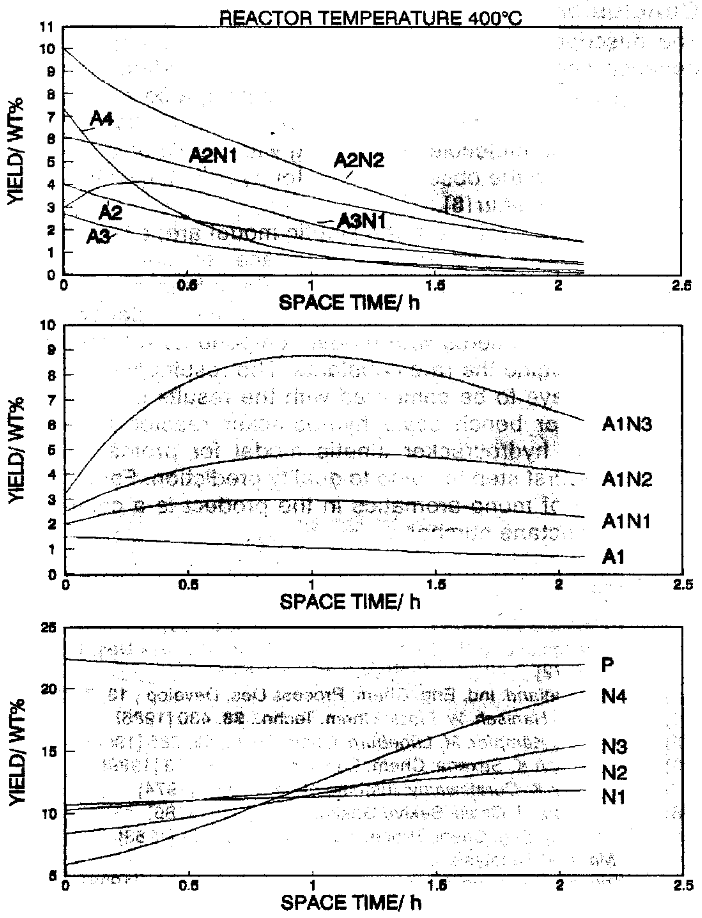

Figure 3: The yield change of 15 pseudo components vs space time. At a reactor space bed temperature of 400 °C

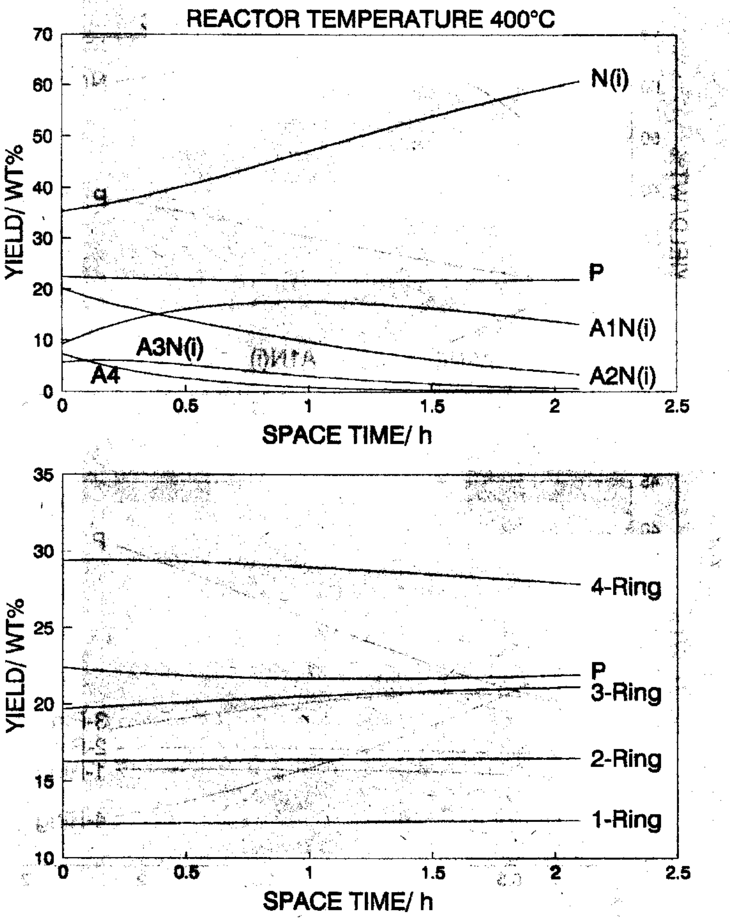

Figure 4: Yield at a reactor temperature of 400 °C

Table III: Detailed analyses of hydrocracker feedstock

Component	Fresh feed [wt%]	Recycle feed [wt%]	Pseudo-component	Feed composition used in the kinetic model [wt%]
5^+ ring aromatics	1.9	5.1		
5^+ ring naphthenes	–	10.4		
4 ring aromatics	2.6	2.9	A_4	7.3
4 ring naphthenes	4.4	11.9	N_4	5.9
3 ring aromatics	5.9	4.7	A_3N_1	3.0
			A_3	2.7
3 ring naphthenes	7.5	11.9	N_3	8.4
2 ring aromatics	22.7	9.0	A_2N_2	10.0
			A_2N_1	6.1
			A_2	4.0
2 ring naphthenes	9.7	12.5	N_2	10.3
1 ring aromatics	10.4	4.2	A_1N_3	3.2
			A_1N_2	2.5
			A_1N_1	2.0
			A_1	1.5
1 ring naphthenes	10.8	10.4	N_1	10.7
Paraffins	23.8	17.0	P	22.4

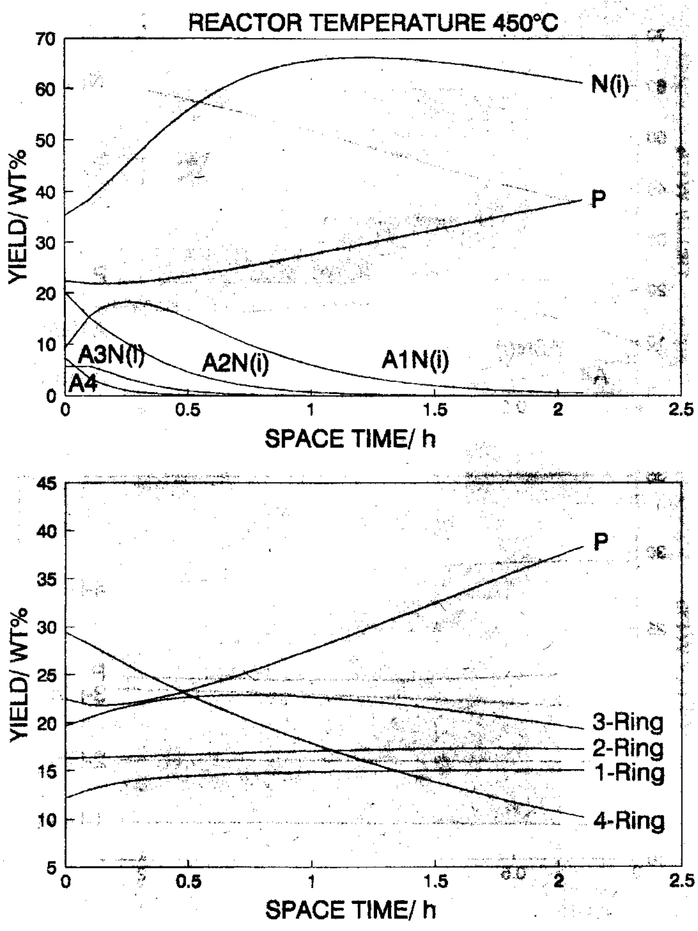

Figure 5: Yield at a reactor temperature of 450 °C

Table IV: The applied Arrhenius equation in the developed model

Reaction			Rate constant equation [h^{-1}]
hydrogenation			
A_4	→	A_3N_1	$K_1 = 2.97\ 10^8 \cdot e^{-105/(RT)}$
A_3N_1	→	A_2N_2	$K_2 = 2.82\ 10^8 \cdot e^{-105/(RT)}$
A_2N_2	→	A_1N_3	$K_3 = 2.54\ 10^8 \cdot e^{-105/(RT)}$
A_1N_3	→	N_4	$K_4 = 1.33\ 10^8 \cdot e^{-105/(RT)}$
A_3	→	A_2N_1	$K_5 = 2.03\ 10^8 \cdot e^{-105/(RT)}$
A_2N_1	→	A_1N_2	$K_6 = 1.52\ 10^8 \cdot e^{-105/(RT)}$
A_1N_2	→	N_3	$K_7 = 1.06\ 10^8 \cdot e^{-105/(RT)}$
A_2	→	A_1N_1	$K_8 = 9.58\ 10^7 \cdot e^{-105/(RT)}$
A_1N_1	→	N_2	$K_9 = 7.67\ 10^7 \cdot e^{-105/(RT)}$
A_1	→	N_1	$K_{10} = 5.36\ 10^7 \cdot e^{-105/(RT)}$
cracking			
A_3N_1	→	A_3	$K_{11} = 1.52\ 10^{15} \cdot e^{-209/(RT)}$
A_2N_2	→	A_2N_1	$K_{12} = 1.22\ 10^{15} \cdot e^{-209/(RT)}$
A_1N_3	→	A_1N_2	$K_{13} = 0.54\ 10^{15} \cdot e^{-209/(RT)}$
N_4	→	N_3	$K_{14} = 2.75\ 10^{13} \cdot e^{-190/(RT)}$
A_2N_1	→	A_2	$K_{15} = 0.36\ 10^{15} \cdot e^{-209/(RT)}$
A_1N_2	→	A_1N_1	$K_{16} = 0.32\ 10^{15} \cdot e^{-209/(RT)}$
N_3	→	N_2	$K_{17} = 2.20\ 10^{13} \cdot e^{-190/(RT)}$
A_1N_1	→	A_1	$K_{18} = 0.29\ 10^{15} \cdot e^{-209/(RT)}$
N_2	→	N_1	$K_{19} = 1.90\ 10^{13} \cdot e^{-190/(RT)}$
N_1	→	P	$K_{20} = 1.60\ 10^{13} \cdot e^{-190/(RT)}$

Conclusion

The description of the individual step results for both hydrogenation and cracking in a first order rate equation in respect to the reactant organic compound, assuming a constant hydrogen concentration and quasi-equilibrium adsorption and desorption of the molecules interacting with the catalyst surface: This is equal to the observed order for hydrocracking by *Qader* [1, 7] and *Hisamitsu* [8].

Two major suppositions in the kinetic model are; all reaction irreversible and a rate controlling surface reaction. These are correct for hydrogen pressures of 15 MPa or higher.

The true rate constant of the reactions in the model are to be identified, experiments with model components will be necessary to determine the rate constants. The results generated by the model have to be compared with the results obtained in a commercial or bench scale hydrocracker reactor. the developed model hydrocracker kinetic model for aromatic feedstocks is the first step to come to quality prediction. For instance the content of mono-aromatics in the product is a component with a high octane number.

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Nomenclature

A	Aromatic	
C_t	Total active hydrogenation sites	mol/m^3 catalyst
C_t^*	Total active cracking sites	mol/m^3 catalyst
C_v	Vacant hydrogenation sites	mol/m^3 catalyst
C_v^*	Vacant cracking sites	mol/m^3 catalyst
ΔE	Activation energy	J.mol^{-1}
K_A	Equilibrium constant of the reactant molecules	
K_H	Equilibrium constant of hydrogen	
K_s	Surface reaction constant	h^{-1}
$K_{c,obs}$	Observed cracking constant	h^{-1}
$K_{HC,obs}$	Observed hydrocracking constant	h^{-1}
$K_{h,obs}$	Observed hydrogenation constant	h^{-1}
$M_{w,i}$	Molar weight	g.mol^{-1}
N	Naphthene	
$-r$	Reaction rate equation	mol.l^{-1}.h^{-1}
$-r_h$	Reaction rate equation due to hydrogenation	mol.l^{-1}.h^{-1}
$-r_c$	Reaction rate equation due to cracking	mol.l^{-1}.h^{-1}
R	Ideal gas law constant	J.mol^{-1}.K^{-1}
S	Hydrogenation site	
S^*	Cracking site	
t	Time	h
T	Absolute temperature	K
y_i	Weight fraction i	wt%
[i]	Concentration of component i	mol.l^{-1}
ρ_f	Specific gravity of the feed	g.ml^{-1}

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