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Kinetic modeling of FCC process

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Abstract

Catalytic cracking of petroleum fractions a process termed as FCC is usually carried out in a reactor block with somewhat complicated hydrodynamic regime. The reactor block is considered as a combination of two different reactors. The riser is a near ideal plug-flow displacement of the catalyst and reaction mixture, while the main reactor vessel (separator) is considered as an ideal mixing CSTR. Temperature gradient along the plug-flow riser can vary on a linear and non-linear dependence. This is reflected by the thermal effect on the cracking products, along the altitude of the riser. Moreover, it can exert a considerable influence on the selectivity of the process in general, as characterized by the diversity of different hydrocarbon groups both in the gaseous and liquid products. The fluid catalytic cracking (FCC) is a process of conversion of a heavy oil fraction into lighter products in a catalytic fluidized reactor. The chemical composition and the structure of the feed are reflected on the catalyst's selectivity and the amount of coke deposited. It is, therefore, necessary to consider the feed type on modeling the process. Cracking reaction in the model was represented as a five-stage process. Reaction rates for the plug-flow riser and the ideal mixing separator are described mathematically in differential and algebraic forms. The model takes into account, exponential dependence of the specific reaction rate on temperature, as well as reflects the influence of the real and bulk catalyst densities, circulation rate, equilibrium and fresh catalyst's activities, reactor pressure, feed rate and unit construction. The model was developed based on a data taken from an industrial FCC unit, that were used to compute the kinetic constants and other parameters. Concrete computed kinetic parameters were compared with corresponding experimental data for adequacy. FCC process is in constant technological development with modernization of especially the riser reactor. Kinetic modeling of the catalytic FCC reactor will give a further understanding of the process and explain the complicated mechanism involved for an efficient and optimal conversion of the feed stock. © 1998 Elsevier Science B.V. All rights reserved.

Keywords: Fluid catalytic cracking; Fluidized reactor; Kinetic modeling

1. Introduction

Fluid catalytic cracking (FCC) is a process in which crude oil fractions are cracked in a riser reactor with a fluidized bed of catalyst. Its mechanism is complicated from both hydrodynamic and chemical points of view. The physical and chemical characteristics of the catalysts (nature, distribution and the structure of the active centers, acid strength etc.) are constantly being modified by the catalyst manufacturers and this makes the process much more difficult. Researchers therefore make a number of assumptions to fit the kinetic equations used in correlation to experimental data.

Nace et al. [1] found Langmuir adsorption appropriate for the kinetic equations and used first order cracking kinetics. Wojciechowsky [2] proposed a three-lump kinetic scheme to account for the conversion of gas oil to gasoline, gas, and coke, and empiri-

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cally determined a cracking termination coefficient. Weekman and Nace carried out similar studies [3]. Catalyst deactivation functions were derived and kinetic equations at steady state operation of the cracking process were proposed by Weekman [4]. Second-order kinetics was considered by Yen et al. [5]. Wallason and others [6] proposed a kinetic model that allows optimization of reactors with boiling bed of catalysts. Kumar et al. [7] developed an integrated FCC reactor–regenerator model utilizing the Weekman 10-lump model.

Mathematical modeling of catalytic cracking becomes much more complicated on considering factors due to macrokinetics. This study gives a descriptive explanation of the stages involved in deriving a kinetic model of a catalytic cracking of crude oil fractions in a fluidized bed of catalyst. Fluidized catalytic cracking of oil fractions with microspherical zeolite-containing aluminosilicate catalysts is an important process in petroleum refineries. Catalytic cracking of oil fractions and regeneration of the spent catalyst is carried out in a reactor–regenerator block.

A sketch of the Russian FCC reactor block, G-43-107, is outlined in Fig. 1. In this study, the reactor block is assumed to be divided into two sections with different hydrodynamic regimes and chemical reaction characteristics. The riser is considered as a plug-flow reactor with ideal displacement of catalyst and reaction mixture. While the main reactor vessel is a continuously stirred tank reactor (CSTR) with ideal mixing. These two regimes are considered separately in modeling the process.

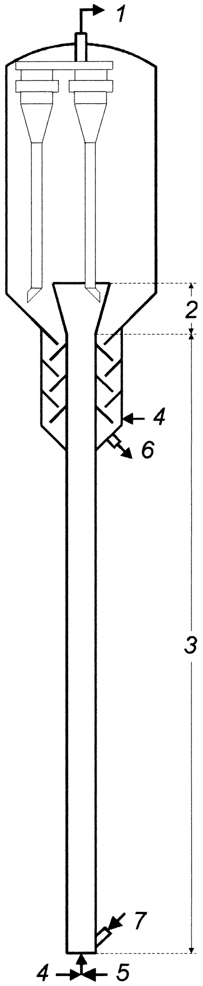

Fig. 1. Reactor-block of the Russian FCC unit. (G-43-107). 1- cracking products; 2- CSTR with ideal mixing; 3- ideal displacing riser reactor; 4- steam; 5- feed; 6- spent catalyst; 7- regenerated catalyst.

2. General kinetic scheme of the catalytic process

Vacuum gas oil, atmospheric distillates, kerosene-gas oil fractions and other crude oil fractions are usually catalytically cracked in a high conversion process to form a complex mixture of gases, and light and heavy fractions. Coke formed in the reaction is deposited on the catalyst, blocking the internal and the external surface and resulting in a substantial reduction in the catalyst's activity. The coke is burned in the regenerator to restore the catalyst activity. The other fractions are passed to fractionator for physical separation.

The general pattern of the FCC product yields clearly indicate that gasoline and distillate increase to maximum and then decline while the amount of coke deposited on the catalyst increases through the reaction. We propose a kinetic scheme with five stages. Products of the vacuum gas oil cracking are lumped in the model and identified as follows: A_1 – feed (heavy oil fraction); A_2 – lighter oil fraction; A_3 – gasoline; A_4 – butane–butene fraction; A_5 – propane–propylene fraction; A_6 – dry gases; A_7 – coke. Kinetics of the catalytic process can be represented schematically as:

$$\begin{aligned}
&A_1 \xrightarrow{k'_1} \upsilon'_2 A_2 + \upsilon'_3 A_3 + \upsilon'_4 A'_4 + \upsilon'_5 A_5 + \upsilon'_6 A_6 + \upsilon'_7 A_7\\
&A_2 \xrightarrow{k''_2} \upsilon''_3 A_3 + \upsilon''_4 A_4 + \upsilon''_5 A_5 + \upsilon''_6 A_6 + \upsilon''_7 A_7\\
&A_3 \xrightarrow{k'''_3} \upsilon'''_4 A_4 + \upsilon'''_5 A_5 + \upsilon'''_6 A_6 + \upsilon'''_7 A_7\\
&A_4 \xrightarrow{k''''_4} \upsilon''''_5 A_5 + \upsilon''''_6 A_6 + \upsilon''''_7 A_7\\
&A_5 \xrightarrow{k'''''_5} \upsilon'''''_6 A_6 + \upsilon'''''_7 A_7
\end{aligned} \tag{1}$$

Where K_i^j is the rate constant of the *i*th component at the *j*th stage and υ_i^j a stoichiometric coefficient of the corresponding stage.

These assumptions about the catalytic process are consistent with the observations where a decrease in the concentration of the feed with time is accompanied by a monotonic increase of products other than gasoline. Fig. 2 gives an example of the behavior calculated by the model. The proposed scheme assumes the following reaction mechanism:

1. Heavy gas oil A_1 is converted to light gas oil A_2, gasoline A_3, lighter hydrocarbon gases A_4–A_6 and coke A_7.
2. Light gas oil A_2 is further cracked to gasoline, light hydrocarbon gases and coke.
3. Gasoline fraction is converted to light hydrocarbon gases and coke.
4. Light hydrocarbon gases (butane–propylene fractions) are partially converted to drier light hydrocarbon gases and coke.
5. Part of the light hydrocarbon gases disintegrates to lighter methane, ethane–ethylene fractions and coke.

The proposed kinetic scheme account for the decline in the concentration of the feed in the products with decrease in molar feed rate, while yielding maxima in the concentrations of A_2 and A_3 and monotonic increases in A_4, A_5, A_6 and A_7. These relationships in the reaction mixture conform to both laboratory and industrial data.

3. Reactor kinetics

As mentioned earlier, the reactor is modeled in two distinct operating regimes. The following assumptions were made on developing the mathematical model of the reactor:

1. Reactor hydrodynamics are first plug-flow and then ideally mixed.

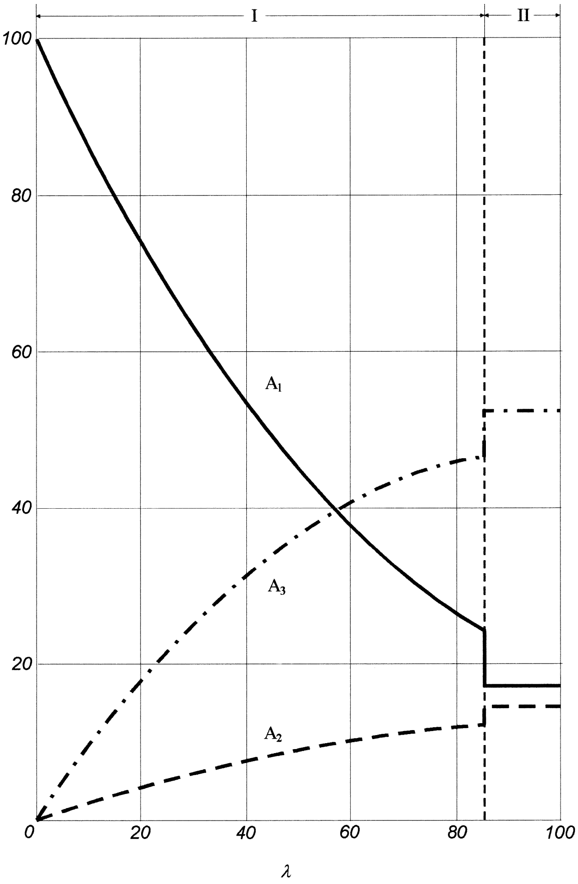

Fig. 2. Numerical values of product's yield at relative reactor length, λ. I-plug-flow riser; II-CSTR.

2. Reactants obey Langmuir's adsorption isotherm.
3. Reactants are weakly and uniformly absorbed on a surface of catalyst with uniformly distributed active centers.
4. Effects of macrokinetics on the cracking rate are neglected.

Reaction rates for the corresponding stages are:

$$\begin{aligned}
\omega_1 &= -k'_1\sigma_1\\
\omega_2 &= v'_2k'_1\sigma_1 - k'_2\sigma_2\\
\omega_3 &= v'_3k'_1\sigma_1 + v''_3k'_2\sigma_2 - k'_3\sigma_3\\
\omega_4 &= v'_4k'_1\sigma_1 + v''_4k'_2\sigma_2 + v''_4k'_3\sigma_3 - k'_4\sigma_4\\
\omega_5 &= v'_5k'_1\sigma_1 + v''_5k'_2\sigma_2 + v'''_5k'_3\sigma_3 + v''''_5k'_4\sigma_4 - k'_5\sigma_5\\
\omega_6 &= v'_6k'_1\sigma_1 + v''_6k'_2\sigma_2 + v'''_6k'_3\sigma_3 + v''''_6k'_4\sigma_4 + v'''''_6k'_5\sigma_5\\
\omega_7 &= v'_7k'_1\sigma_1 + v''_7k'_2\sigma_2 + v'''_7k'_3\sigma_3 + v''''_7k'_4\sigma_4 + v'''''_7k'_5\sigma_5
\end{aligned} \tag{2}$$

Feed and reaction products are considered weakly absorbed on the catalyst surface. In addition, the adsorption of each component is in direct proportion to its partial pressure. The adsorption isotherm as expressed by Henry's Law takes a linear form:

$$\sigma_i = b_i p_i \tag{3}$$

The partial pressure of each component is related to the total pressure by Dalton's Law:

$$p_i = p\frac{n_i}{\sum n_i} \tag{4}$$

The catalyst surface area occupied by the ith component can therefore be expressed as a fraction of the total pressure by:

$$\sigma_i = b_i\frac{n_i}{\sum n_i}P \tag{5}$$

Eq. (2) can be rearranged as follows:

$$\begin{aligned}
\omega_1 &= -\frac{P}{\sum n}k'_1 b_1 n_1\\
\omega_2 &= \frac{P}{\sum n}(v'_2 k'_1 b_1 n_1 - k'_2 b_2 n_2)\\
\omega_3 &= \frac{P}{\sum n}(v'_3 k'_1 b_1 n_1 + v''_3 k'_2 b_2 n_2 - k'_3 b_3 n_3)\\
\omega_4 &= \frac{P}{\sum n}(v'_4 k'_1 b_1 n_1 + v''_4 k'_2 b_2 n_2 + v'''_4 k'_3 b_3 n_3 + -k'_4 b_4 n_4)\\
\omega_5 &= \frac{P}{\sum n}(v'_5 k'_1 b_1 n_1 + v''_5 k'_2 b_2 n_2 + v'''_5 k'_3 b_3 n_3 + v''''_5 k'_4 b_4 n_4 - k'_5 b_5 n_5)\\
\omega_6 &= \frac{P}{\sum n}(v'_6 k'_1 b_1 n_1 + v''_6 k'_2 b_2 n_2 + v'''_6 k'_3 b_3 n_3 + v''''_6 k'_4 b_4 n_4 + v'''''_6 k'_5 b_5 n_5)\\
\omega_7 &= \frac{P}{\sum n}(v'_7 k'_1 b_1 n_1 + v''_7 k'_2 b_2 n_2 + v'''_7 k'_3 b_3 n_3 + v''''_7 k'_4 b_4 n_4 + v'''''_7 k'_5 b_5 n_5)
\end{aligned} \tag{6}$$

The above equations are a generalized kinetic scheme for the catalytic process. The kinetic equations depend on the type of reactor regime to be considered.

3.1. The CSTR reactor vessel

The portion of the reactor vessel considered being the CSTR, a well-mixed isothermal mixture of products and catalyst is assumed. Model kinetic equations of the ideal mixing regime are characterized in the reactor vessel by an instantaneous mixing of hydrocarbon vapors and the catalyst and, therefore, include only a material balance. Generally, a component continuity equation of an ideally mixed heterogeneous catalytic chemical process may be written as:

$$\frac{\mathrm{d}(C_i V)}{\mathrm{d}t} = C_i^0 V_1 - C_i V_2 + \omega_i S \tag{7}$$

For gaseous reaction mixtures in a stationary regime, Eq. (7) may be reduced to a form:

$$\omega_i = \frac{C_i V_2 - C_i^0 V_1}{S} \tag{8}$$

Concentration of the ith component at the entrance and the outlet can be expressed as $C_i^0 = n_i^0/V_1$ and $C_i = n_i/V_2$, respectively. An expression for the reaction rate taking into consideration a unit length of the reactor ℓ can be written as:

$$\omega_i = \frac{\Delta n_i}{S\ell} \tag{9}$$

where, $\Delta n = n_i - n_i^0$

Assuming a constant feed flow rate ($n_i^0 = \text{const.}$), constant reactor pressure and a stable catalyst activity. We may substitute as follows:

$$B = \frac{PS\ell}{n_i^0}k'_1 b_1 \tag{10}$$

$$k_i = \frac{k'_i b_i}{k'_1 b_1} \tag{11}$$

Then, for practical purposes, Eq. (6) may be rearranged as:

$$
\begin{array}{ll}
(1+Bk_1)N_1 & =1 \\
Bv'_2k_1N_1-(1+Bk_2)N_2 & =0 \\
Bv'_3k_1N_1+Bv''_3k_2N_2-(1+Bk_3)N_3 & =0 \\
Bv'_4k_1N_1+Bv''_4k_2N_2+Bv'''_4k_3N_3-(1+Bk_4)N_4 & =0 \\
Bv'_5k_1N_1+Bv''_5k_2N_2+Bv'''_5k_3N_3+Bv''''_5k_4N_4-(1+Bk_5)N_5 & =0 \\
Bv'_6k_1N_1+Bv''_6k_2N_2+Bv'''_6k_3N_3+Bv''''_6k_4N_4+Bv'''''_6k_5N_5-N_6 & =0 \\
Bv'_7k_1N_1+Bv''_7k_2N_2+Bv'''_7k_3N_3+Bv''''_7k_4N_4+Bv'''''_7k_5N_5-N_7 & =0
\end{array}
\qquad (12)
$$

where, $N_i = n_i/\sum n_i$, the molar fraction of the *ith* component in the mixture.

Eq. (12) given above, is a mathematical expression of catalytic processes in a CST reactor vessel assuming a near isothermal regime.

3.2. The ideal plug-flow riser

The reaction mixture of oil and catalyst from the mix zone to the riser outlet is in a regime closer to plug-flow. Conversion at equivalent conditions is then a function of the riser's dimensions.

The reaction rate equation for a plug-flow riser can be written as:

$$\frac{\mathrm{d}n_i}{S\mathrm{d}\ell} = \omega_i \qquad (13)$$

In analogy to (Eq. (6)) the kinetic equation of a FCC riser with plug-flow displacement of reaction mixture and the catalyst is contained in (Eq. (14)). Eliminating back-mixing, with concentration varying only along the length gives a kinetic equation for the riser of:

$$
\begin{array}{l}
\frac{\mathrm{d}N_1}{\mathrm{d}\lambda} = -BN_1 \\
\frac{\mathrm{d}N_2}{\mathrm{d}\lambda} = B(v'_2N_1 - k_2N_2) \\
\frac{\mathrm{d}N_3}{\mathrm{d}\lambda} = B(v'_3N_1 + v''_3k_2N_2 - k_3N_3) \\
\frac{\mathrm{d}N_4}{\mathrm{d}\lambda} = B(v'_4N_1 + v''_4k_2N_2 + v'''_4k_3N_3 - k_4N_4) \\
\frac{\mathrm{d}N_5}{\mathrm{d}\lambda} = B(v'_5N_1 + v''_5k_2N_2 + v'''_5k_3N_3 + v''''_5k_4N_4 - k_5N_5) \\
\frac{\mathrm{d}N_6}{\mathrm{d}\lambda} = B(v'_6N_1 + v''_6k_2N_2 + v'''_6k_3N_3 + v''''_6k_4N_4 + v'''''_6k_5N_5) \\
\frac{\mathrm{d}N_7}{\mathrm{d}\lambda} = B(v'_7N_1 + v''_7k_2N_2 + v'''_7k_3N_3 + v''''_7k_4N_4 + v'''''_7k_5N_5)
\end{array}
\qquad (14)
$$

where, $\lambda = l/l_0$ is the relative length of the reactor, and l_0 is the total length of the 'combined' reactor.

Eq. (14) is a mathematical expression of the catalytic processes in the plug-flow riser. Its solution will give the concentration of each respective component at any distance from the reactor inlet. Fig. 2 illustrates the product distribution along the relative length of the reactor and the two regimes (plug-flow and CSTR) can be distinctly noticed.

4. Model's parameters and temperature relation

Changing the reaction temperature will change the numerical values of the parameters that determine the kinetics of the process in general. In the model temperature-dependent parameters are contained in the constant B introduced in Eq. (10):

$$B = \frac{PS\ell}{n_1^0} k'_1 b_1$$

k'_1 and b_1 are the most temperature sensitive factors in parameter 'B'. The adsorption coefficient b_1 is a ratio of absorption rate constant k_1 to desorption rate constant k_2; $(b_1 = k_1/k_2)$.

The adsorption coefficient 'b_1' can be expressed as:

$$b_1 = \frac{C_1\sqrt{T}}{C_2 \mathrm{e}^{-\Delta H/RT}} \qquad (15)$$

Moreover, the cracking rate constant may be determined as;

$$k = C_3 \mathrm{e}^{-E/RT} \qquad (16)$$

The parameter B can then be expanded to:

$$B = \frac{PS\ell}{n_1^0} k_1^0 \sqrt{T} e^{-E^*/RT} \qquad (17)$$

Where $E^* = E - \Delta H$ and $k_1^0 = C_1C_3/C_2$ a constant that sorely depends on the nature of the catalyst.

Parameter B is an important parameter for reactor design. Note that conversion is proportional to this

Table 1
Model's calculated kinetic constants

Parameter *B*,	0.0322
Activation energy, cal/mol. K	2.38 E +04
Frequency factor, *k*, mol./ at.h	1.33 E +04
Correction coefficient	0.40

Stoichiometric coefficients

Product index/stage number

2	1	2	3	4	5
3	0.133				
3	0.618	0.194			
4	0.076	0.106	0.235		
5	0.077	0.335	0.495	0.358	
6	0.445	0.203	0.241	0.235	0.434
7	0.050	0.161	0.029	0.407	0.566
	1.000	1.00	1.00	1.00	1.00
Rate constants, k_j					
	1.00E+00	6.63E-07	7.54E-06	2.45E-03	3.72E-03

parameter. The derived equations can be applied to the case of a FCC unit operating in a steady state. Model kinetic constants and other parameters are computed for a given feed stock under certain technological conditions. Results of such calculations are given in Table 1.

5. Results and discussion

The model's adequacy was checked against the performance of industrial Russian FCC unit (G-43-107) at the Moscow refinery. Experimental and calculated data are found to be in a good agreement. Examples of the industrial data from this unit are given in Table 2. Data at different temperatures, pressures, feed rates and catalyst activities were used to check the adequacy of the model.

Table 2
Moscow Refinery FCC data for vacuum gas oil cracking

Feed				
Spec. density, kgm^{-3}	894	895	891	—
Sulfur, wt.%	0.63	0.67	0.69	0.66
Feed rate, tonnes/day	3967	4558	4952	5407
Recycle, %	5.7	5.6	5.7	5.1
Riser outlet temp., °C.	511	511	511	511
Catalyst quality				
MAT activity	73.3	72.5	71	70
Surface area, m^{-2}g	110	109	110	110
Catalyst-to-oil ratio	7.47	7.86	6.87	7.19
Products yield, wt.%				
Dry gas	4.72	3.93	4.01	3.57
Gasoline	51.42	49.07	48.0	47.7
LCO	14.4	18.0	19.7	22.5
Slurry	6.6	6.9	7.74	9.83
Coke	4.7	4.4	3.7	3.6

5.1. *Feed rate*

An increase in feed rate to the reactor is attended by a decrease in the degree of conversion. This is clearly caused by the inability of the heavy gas oil lump to convert to lower molecular weight products. Introducing a more active catalyst or increasing the regime's temperature may compensate for this loss in conversion. A plot of some of the products yield vs. the reactor feed rate is given in Fig. 3.

5.2. *Nature and density of the charge*

Stocks with different densities were investigated. The composition of the feed and the degree of conversion appear to exert a considerable effect

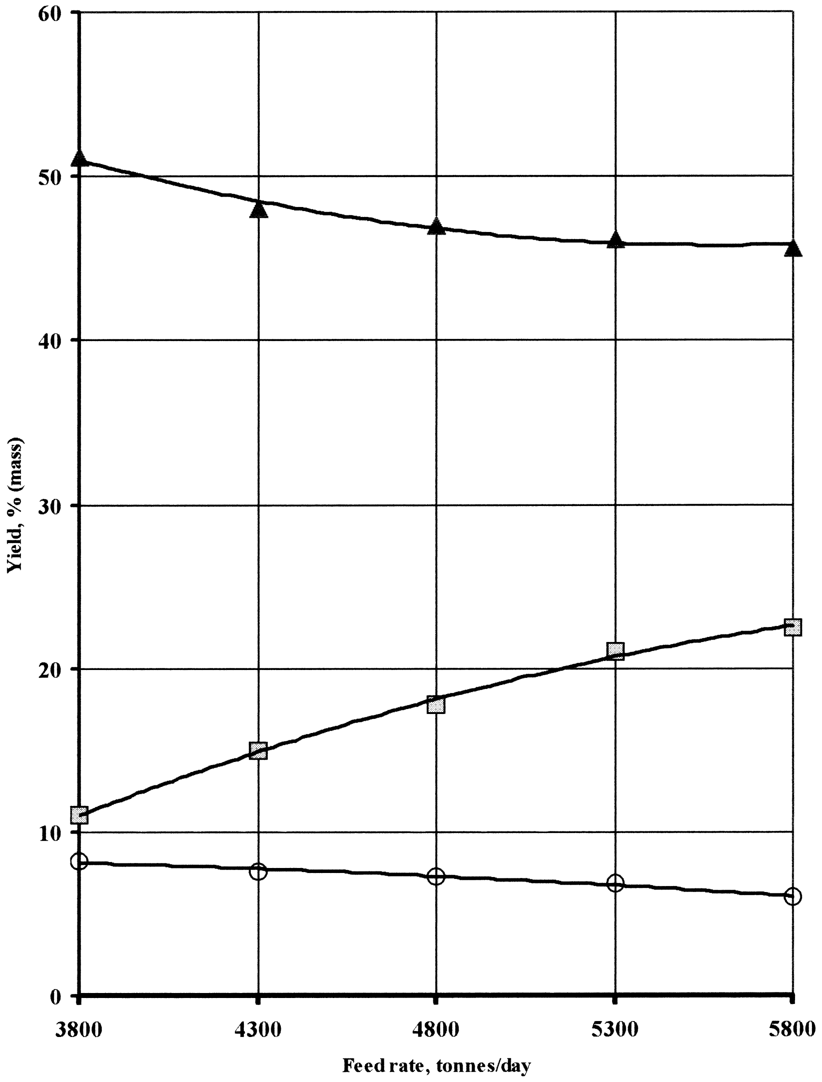

Fig. 3. Effect of feed rate on product yields. (▲), gasoline lump; (□), heavy gas oil fraction; (○), light gas oil fraction. Points are industrial data while curves are the corresponding calculated values.

on the product's yields, the coke yields increase significantly as the density of the feed is increased. At the Moscow refinery, the feed is first hydrofined to lower the amount of sulfur and reduce the contamination of the heavy metals. Thus effect of heavy metals and sulfur were neglected in developing the model. The effect of the quality of the feed on the product yields is shown in Table 3. Paraffinic vacuum gas oils of different origin were fed to the G-43-107 FCC unit at the Moscow refinery. Heavier feeds produced more gasoline. This may be associated with high conversion attained when charging these types of stocks.

5.3. *Reactor temperature*

Increasing the process temperature increases the conversion of the feedstock. Temperatures above

Table 3
Effect of feed density on products yield

Regime conditions					
Riser outlet temperature, °C	512	512	511	512	510
E-catalyst activity	72.3	72.0	72.2	71.5	71
Feed rate, t/d	4700	4693	4632	4602	4587
Catalyst-oil-ratio	6.1	6.1	5.9	5.5	5.5
Density, @20°C, kg/m^3	876	882	889	904	915
IBP	211	214	284	209	265
10%	335	337	350	334	351
50%	411	407	410	412	410
EBP	511	509	510	504	506
Product yields, % mass					
Experimental/calculated					
HGO (A_1)	19.7/21.4	18.3/19.0	17.7/18.5	16.6/17.2	14.9/15.0
LGO (A_2)	13.1/10.5	12.8/11.8	12.3/10.6	11.2/10.7	10.4/11.0
Gasoline (A_3)	48.4/48.1	48.9/48.7	49.8/49.4	50.4/50.0	50.7/50.1
B–B fraction (A_4)	6.3/6.0	7.4/6.9	8.2/7.6	8.7/7.9	9.3/8.5
P–P fraction (A_5)	4.5/5	5.1/5.2	4.9/5.7	5.7/5.8	6.7/6.1
Dry gas (A_6)	4.7/4.5	4.0/4.2	3.5/3.8	3.4/4.1	3.3/4.2
Coke ($A7$)	3.3/3.9	3.5/4.2	3.6/4.4	3.9/4.3	4.7/5.1

525°C noticeably reduce the gasoline yield, and increase the yields of gas and coke. Fig. 4 shows the trends for product's yields from the refinery data and the corresponding calculated values.

Optimal gasoline yield is attainable at 517°C, but this optimum can shift below or above this temperature when other process conditions are altered or the equilibrium catalyst's activity is changed. This sensitivity clearly indicates the complexity of the FCC process and the presence of multiple steady states. The maximum in gasoline yield with increasing temperature may be connected

Table 4
Testing the model with data from Moscow's Refinery FCC unit

Condition	1	2	3	4	5
Operating conditions					
Feed density @ 20°C, kg/m^3	888	891	899	878	894
Feed rate, t/d	5168	5159	4701	5311	4858
Riser outlet temperature, °C	509	511	515	508	513
Reactor pressure, atm.	1.2	1.22	1.17	1.25	1.19
Catalyst-oil-ratio	5.49	5.99	7.0	5.23	6.18
Catalyst properties					
E-activity	71.8	69.5	61	72.5	65
Surface area, m^2/g	111	104	81	117	89
ABD, g/cc	0.93	0.89	0.70	0.90	0.72
Refinery/model					
HGO (A_1)	19.7/18.8	19.7/20.7	26.3/24.8	13.0/14.2	23.0/23.1
LGO (A_2)	10.5/10.7	11.0/10.5	10.6/9.9	11.8/11.4	11.5/10.2
G-line (A_3)	50.9/49.7	48.4/48.5	46.8/46.0	51.9/52.5	47.6/47.0
B–B F (A_4)	6.7/6.0	5.9/6.1	7.6/6.2	9.8/7.0	7.7/6.32
P–P F (A_5)	4.9/6.8	7.8/6.5	3.5/5.7	5.5/6.6	4.9/5.9
Gas (A_6)	3.0/3.8	3.8/3.7	2.0/3.5	4.1/4.0	2.2/3.6
Coke (A_7)	3.9/4.0	3.6/3.9	2.9/3.7	3.5/4.2	3.0/3.7

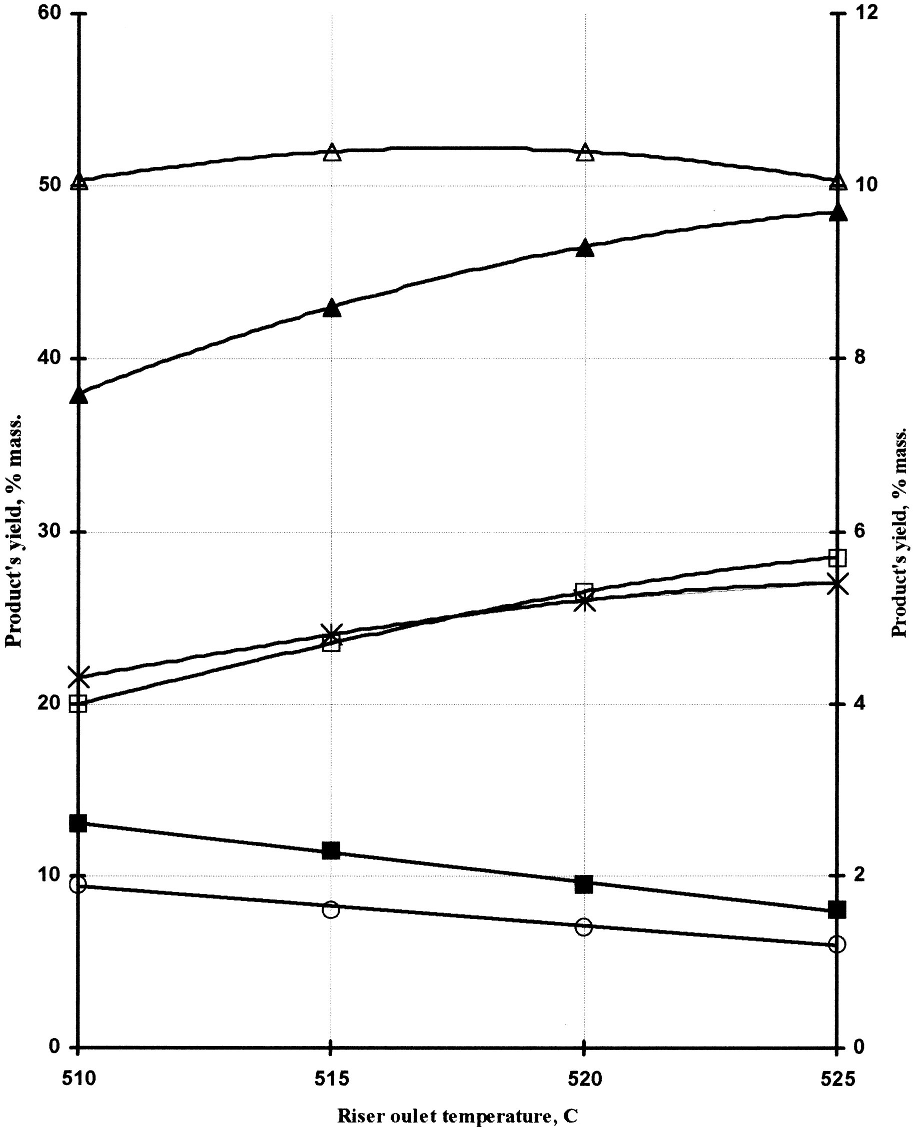

Fig. 4. Effect of temperature on product's yield. Y1-axis (left): (△), A_3 (gasoline lump); (■), A_1 (heavy gas oil fraction); (○), A_2 (light gas oil fraction. Y2-axis (right) (▲), A_4 (butane–butene fraction); (□), A_7 (coke); (×), A_6 (dry gas). Points are industrial data while curves are the corresponding calculated values.

with the instability and further cracking of some of the gasoline lumps.

5.4. Catalyst quality

This work investigated two commercial catalysts with different chemical and physical characteristics and these are compared in Table 4.

5.5. Catalyst-to-oil ratio

An increase in the catalyst-to-oil ratio decreases the residence time of the catalyst in the reaction zone. We noticed a decrease for coke deposited on a particular particle.

The relationship of the catalyst-to-oil to feed conversion and gas yield is shown in Fig. 5. Changing the

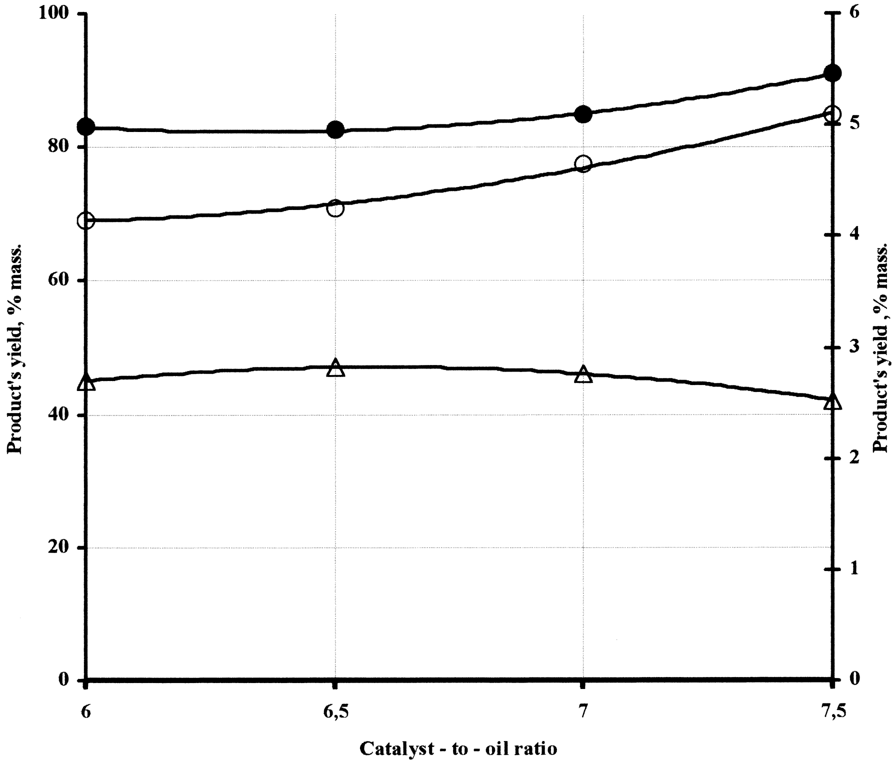

Fig. 5. Effect of catalyst-to-oil ratio on the product's yield. Y1-axis (left): (●), total conversion; (Δ), A_3 (gasoline lump). Y2-axis (right): (○), A_7 (coke). Points are industrial data while curves are the corresponding calculated values.

catalyst-to-oil ratio can regulate the amount of heat introduced to the reactor from the regenerator. Feed conversion as well as the amount of coke deposited on the catalyst can be maintained by changing the catalyst-to-oil-ratio.

The model was implemented in a computer program that serves as a process simulator and optimizer. All the kinetic equations were interconnected, the ideal plug-flow reactor data serves as input for the CSTR vessel. Operators use the model to do the following:

1. Analyze the FCC unit data in order to:

- Establish the mechanism of catalytic cracking in relation to the model,
- Determine the number of stages and compute the kinetic constants of each stage involved,
- Compute stoichiometric coefficients, and
- Determine the optimal regime parameters

2. Predict the product yield using a limited data input,
3. Determine the catalyst coke make-up, and
4. Trouble-shoot the FCC unit.

6. Nomenclature:

k'_j	Rate constant of corresponding stage in the kinetic scheme
ν_i^j	Stoichiometric coefficient of *i*th component at *j*th stage
A_i	Component (fraction) *i*
ω_i	Rate of formation of component *i*
σ_{A_i}	Catalyst's surface occupied by a corresponding component
b_i	Adsorption coefficient
n_i	Number of moles of *i*th component

C_i^0, C_i	Inlet and outlet concentration of an *i*th fraction in the reactor
$V_1 V_2$	Feed rates
V	Catalyst-free reactor volume
$\mathrm{C}_1,\mathrm{C}_2,\mathrm{C}_3$	Constants
k_i^0	Constant determined by the nature of the feed
E	Activation energy
ΔH	Heat of adsorption
R	Universal gas constant
ℓ	Length (coordinate)
S	Catalyst surface area

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