TOMSK POLYTECHNIC UNIVERSITY

# MATHEMATICAL MODELING OF VACUUM GAS OIL CATALYTIC CRACKING FROM WEST SIBERIAN AND KAZAKHSTAN OIL BLEND


G.Y. Nazarova[1], E.N. Ivashkina[1], E.D. Ivanchina[1], A.A. Oreshina[1], G.R. Burumbaeva[2], G.Z. Seitenova[3], T.A. Kaliev[2,3]

[1]Tomsk Polytechnic University, silko@tpu.ru

[2] LLP Pavlodar Petrochemical Plant

[3] S. Toraighyrov Pavlodar State University


## INTRODUCTION

Depending on market needs, the catalytic cracking technology can be aimed at in-creasing the yield of gasoline, light olefins or light gasoil, the latter being more relevant to Europe with its high amount of diesel cars. Factors affecting the products yields include interacting operating variables in the reactor and the regenerator, catalyst de-activation, and, especially, change in the hydrocarbon type content in the feedstocks.

When the heavy petroleum fractions are converted, the rising the content of coke on the catalyst contributes to its deactivation and an increase in the temperature of the regenerated catalyst. In this case, the amount of heat created in the regenerator should not deactivate the catalyst or disturb the heat balance significantly. At the same time, the conversion of catalytic cracking feedstock is limited by the regenerator coke burning ability.

Comprehensive feed research, development and application of a mathematical model make it possible to assess the possibility of using a different composition of the feedstock and to determine the cracking temperatures which is required to fuels and petrochemical modes taking into account the feedstock composition.

A mathematical model of catalytic cracking on the basis of the thermodynamic and kinetic as well as the catalyst deactivation patterns was developed in this study. The influence of the feedstock types on the yield of catalytic cracking products, the fuel and petrochemical mode as well as the degree of catalyst deactivation have been determined. Among the studied types of raw materials are mixtures of Kazakh and West Siberian oil.

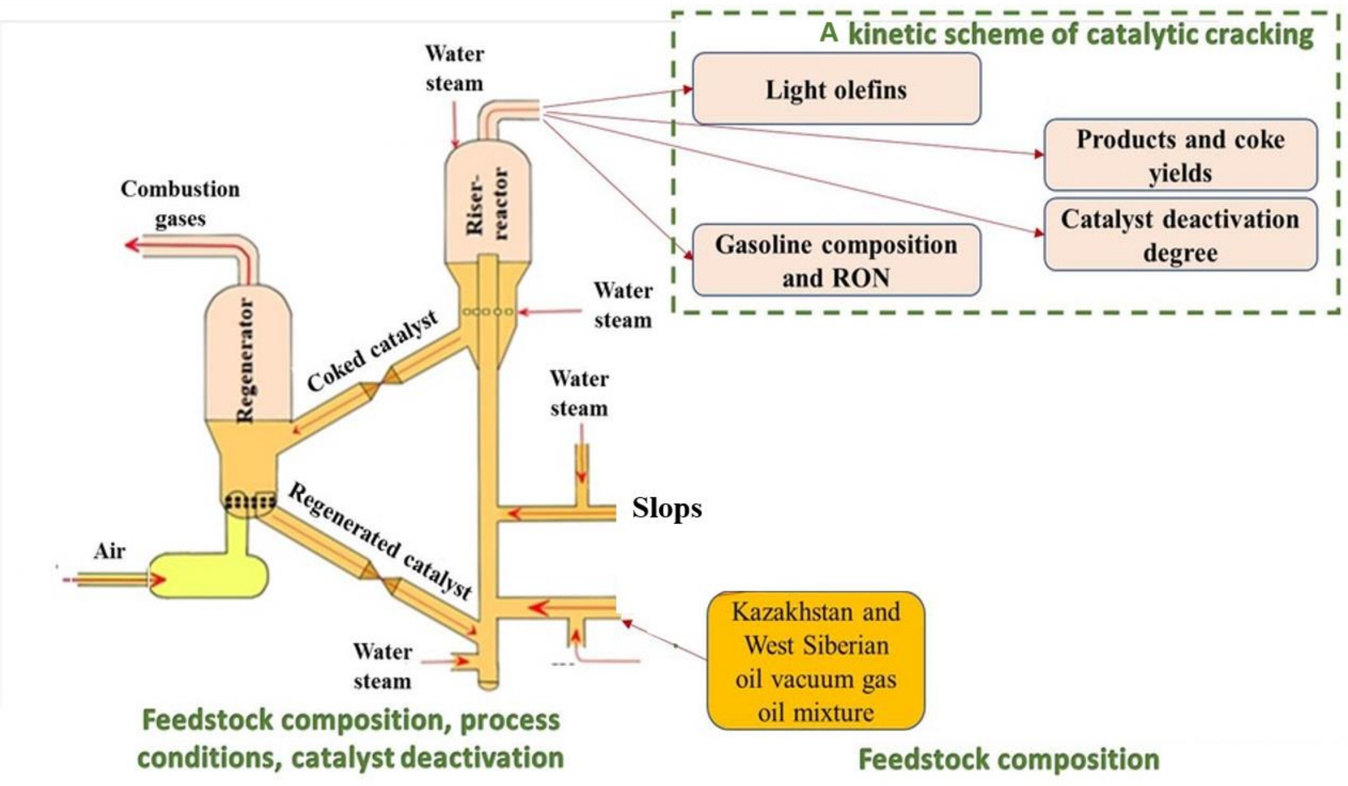


**Fig. 1. The block diagram of catalytic cracking unit.**

## MATHEMATICAL MODELLING

### Model equation

$$\begin{cases} \dfrac{dC_i}{d\tau} = \sum_{j=1}^{18} (\pm\psi \cdot (W_j - W_{-j})) \\ \rho_{cm} c_{cm} \dfrac{dT}{d\tau} = \sum_{j=1}^{18} (\pm\psi \cdot ((\Delta_r H_T^\circ)\cdot W)_j - ((\Delta_r H_T^\circ)\cdot W)_{-j})) \end{cases}$$

**Table 1. Feedstock composition to model calculation**

| Groups | Content, %мас. | | | | | | |
|---|---|---|---|---|---|---|---|
| | №1 | №2 | №3 | №4 | №5 | №6 | №7 |
| Saturates | 57.7 | 59.0 | 61.6 | 63.5 | 66.0 | 72.6 | 73.1 |
| Aromatics | 39.7 | 36.6 | 35.4 | 33.9 | 30.1 | 25.1 | 23.3 |
| Resins | 2.6 | 4.4 | 3.0 | 2.6 | 4.0 | 2.3 | 3.6 |

The catalyst dehydrogenation ability and deactivation function: $A = A_0 \cdot \exp(-k_d \cdot C_k)$ $\gamma = \exp(k_{H2} C_{Ni})$

Initial conditions: $C_i = C_{i,0}$, $T0 = T_{i.t.}$ $\tau$ is the contact time, s; j is the reaction number; $p_m$, $c_m$ are the density and heat capacity of flow, kg/m³, kJ / kg · K; $C_i$ is the concentration of i-the hydrocarbons group, mol/m³; ψ is the deactivation function; A is the current relative catalyst activity, %; $A_0$ is regenerated catalyst activity, %; $C_{coke}$ is the coke content on the catalyst, wt%; $\gamma$ – catalyst dehydrogenation ability; $k_d$ – deactivation constant; $k_{H2}$ – dehydrogenation constant; T is the temperature; $T_{i.t.}$ is the initial temperature of cracking, K;

$\vec{W}$, $\overleftarrow{W}$ are the reaction rate in the forward and reverse directions, mol/(s·m³); $\Delta r \vec{H}_T^\circ$, $\Delta r \overleftarrow{H}_T^\circ$ are the thermal effects of the chemical reactions, kJ/mol;

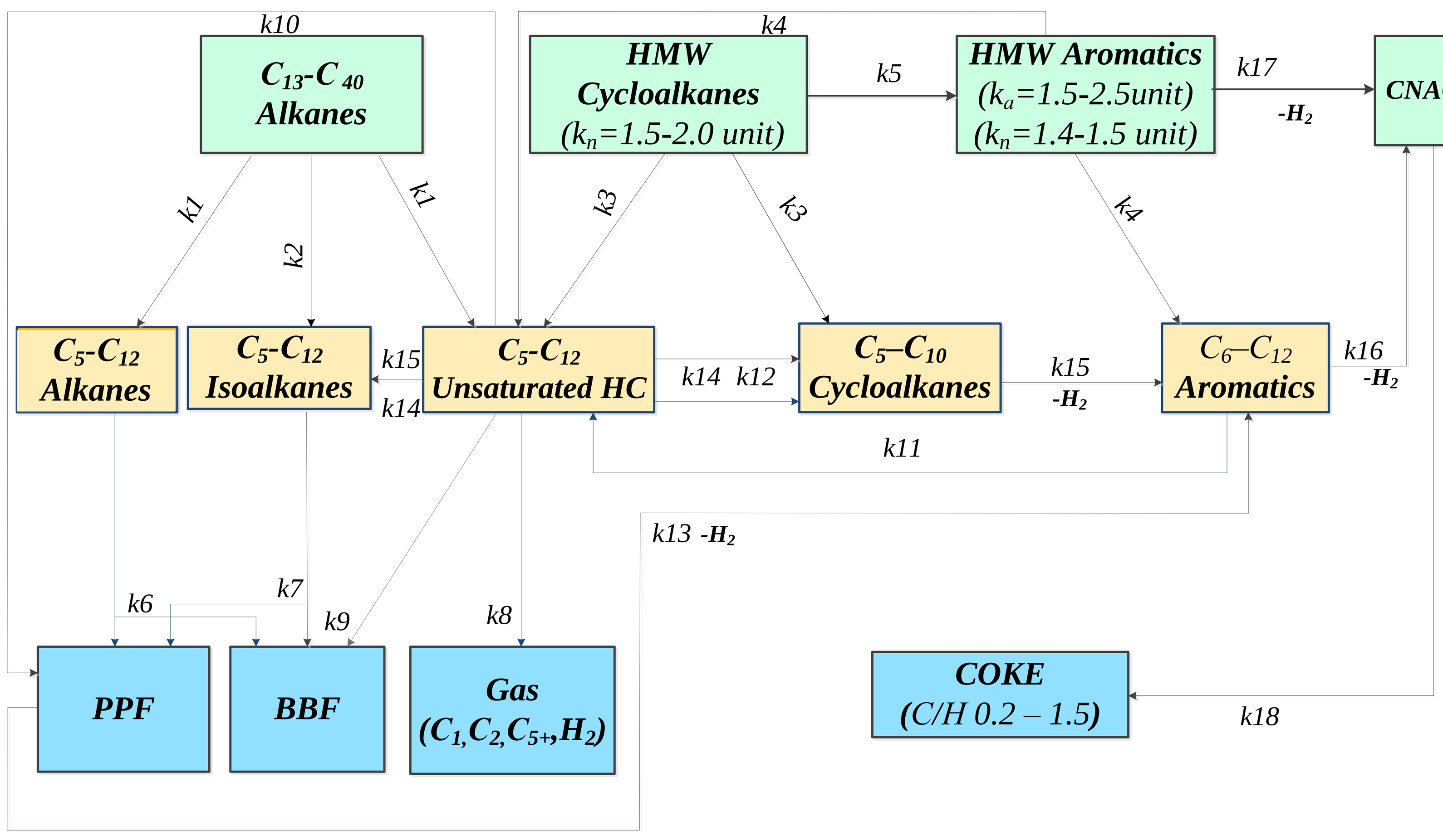


**Fig. 2. A kinetic scheme of catalytic cracking reactions at temperature of 810-848 K**

### Feedstock-induced changes

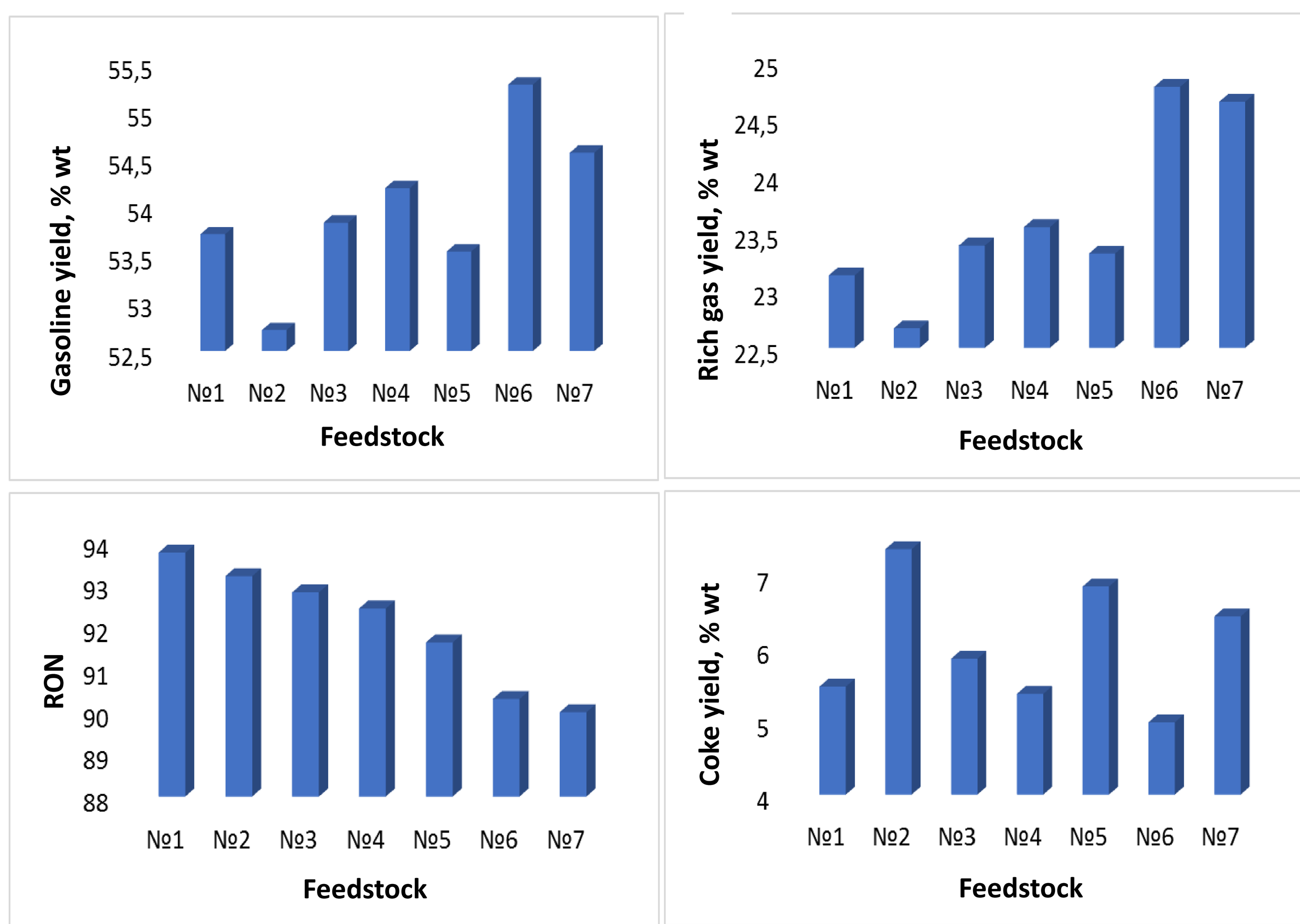


**Fig. 3. Feedstock-induced change on the products yields**

### Process variables

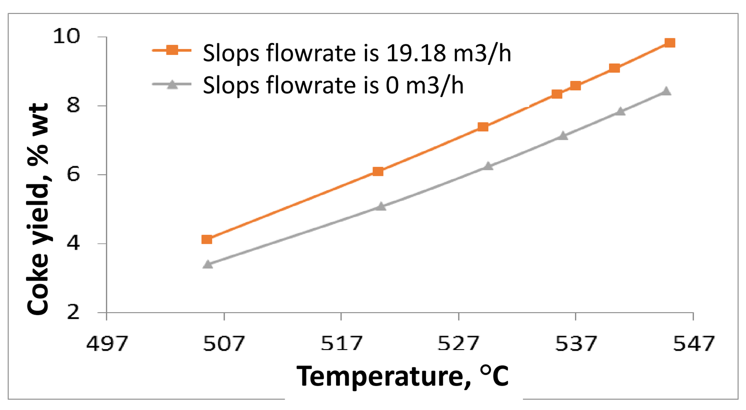


**Fig. 5. Coke yield depending on the slops flowrate**

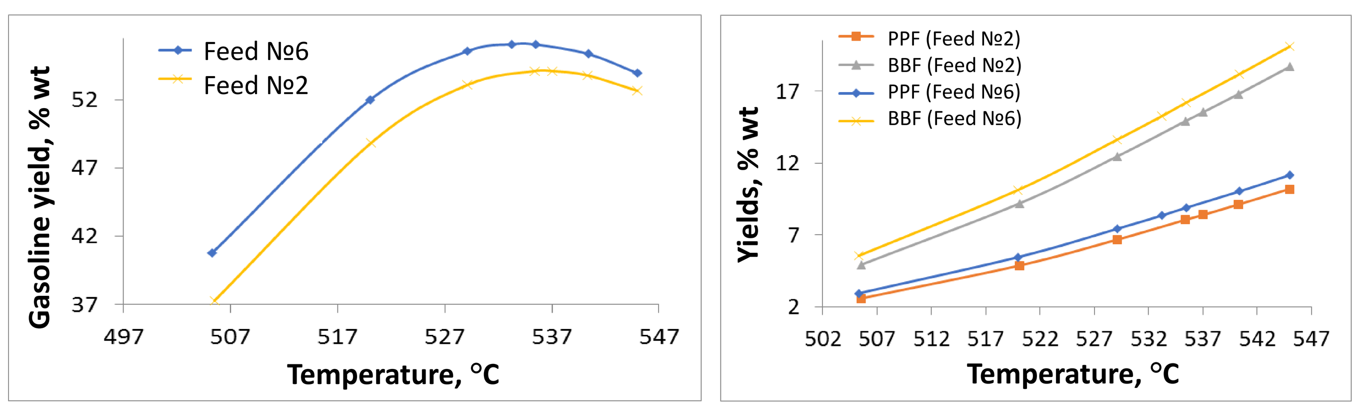


**Fig. 4. A target product yields depending on the cracking temperature**

## RESULTS AND DISCUSSION

The fuel operating modes of the catalytic cracking riser (Table 3) have been determined for three feedstock types, which ensure the maximum gasoline yield (52.6–56.1 wt% (1648.3–1744.7 tons/day)).

The maximum gasoline yield is achieved without any significant restrictions when feedstock № 6 and №5. At the same time, a highly resinous feedstock (№2) requires to reduce the slops flowrate to riser in order to reduce the coke load on the regenerator and prevent catalyst thermal destruction.

The petrochemical mode, when the highly paraffinic feedstock (No. 6) is converted, is ensured at 534–545 ºC, the yield of PPF and BBF are 8.4–11.2 and 15.3–20.1 wt%. in the specified temperature range. This corresponds to 261.2–348.3 and 475.8–625.1 tons/day.

A petrochemical mode to produce a hight amount of light olefins do not be achieved when a highly aromatic and resinous feedstock No. 2 converts due to a significant restrictions by coke.

When the feedstock with a high content of saturates and resins (№ 5) is converted, it is necessary to stop the slops flowrate to riser. This stems from increasing in the "rigidity" of the process contributes to intensive coke formation. The maximum PPF and BBF for feedstock № 5 are 8.3–10.3 and 15.2–18.6% wt. (258.2–320.3 and 472.7–569.1 tons / day) when the temperature was 536–545 ºC.

Thus, the use of a mathematical model, which is based on the phyco-chemical patterns and took into account the reactions leading to the coke formation, provides a forecast of the yield and quality of the products depending on the feedstock composition and process variables.

Table 4. Components not involved in the production of gasolines

| Показатель | Сырье №6 | | Сырье №5 | | Сырье №2 | |
|---|---|---|---|---|---|---|
| Целевой продукт | Бензин | ППФ и ББФ | Бензин | ППФ и ББФ | Бензин | ППФ и ББФ |
| Температура крекинга, ºС | 533 | 534–545 | 535,5 | 536–545 | 537 | – |
| Расход шлама, м³/ч | 19,18 | | 19,18 | 0 | 0 | – |
| Выход, % мас (тн/сут): – бензинаА – ППФ –ББФ | 56,1 (1744,7) | 8,4–11,2 (261,2–348,3) 15,3–20,1 (475,8–625,1) | 54,66 (1699,9) | 8,3–10,3 (258,2–320,3) 15,2–18,6 (472,7–569,1) | 52,6 (1648,3) | – |
| Выход кокса, % мас. | 5,5 | 5,5–7,0 | 7,7 | 6,8–7,7 | 7,4 | – |