Petroleum and Coal

Article **Open Access**

OPTIMAL DESIGN OF STRAIGHT– RUN GASOLINE CONVERSION ON ZEOLITE CATALYST

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Received September 9, 2016; Accepted November 2, 2016

Abstract

The HYSYS Aspen Plus software is used to develop a model of the reactor unit including a plug flow reactor and distillation sequence for conversion of gasoline fractions. The constructive and process variables of the key equipment were optimized stepwise with the model. The developed objective dimensionless function allows choosing optimal conditions for work in the mode of maximum yield or in the mode of maximum octane number of the product. The reactor was designed and optimal modes were found for both the reactor and fractionation unit.

Keywords: zeolite catalyst; kinetic modeling; plug flow reactor; distillation sequence; optimal modes; objective dimensionless function.

1. Introduction

As compared to the technologies based on hydrogen and expensive platinum catalysts usage, zeolite catalysts have a number of advantages:

- Greater thermal and mechanical stability;
- High selectivity;
- Low operating costs and investments;
- Freedom from hydrotreating.

A variety of studies has been conducted in hydrocarbon processing on zeolite as catalysts or as carriers of catalysts. The studies of heavy hydrocarbons cracking on zeolite to produce the high–octane components of gasoline were presented in [1–3].

The authors of [4-5] have studied alkylation of benzene with ethylene on zeolite catalyst. They noted technology simplification, reducing operating costs of feed preparation, and neutralization of acid waste water.

CLG (USA) in collaboration with Akzo Nobel (Netherlands) developed the "Alky – Clean" – process of isoparaffin alkylation with olefins on solid acid zeolite catalysts [6] for production of high–octane aromatics and sulfur free alkylation gasoline. The "BIMT" technology of straight –run gasoline conversion to high–octane gasoline on zeolite catalysts was developed at Boreskov Institute of Catalysis [7].

Design of industrial units based on laboratory investigations includes scaling and optimization. The model simulating these processes will enable:

- Cutting scaling time and number of stages;
- Optimization of the constructive and process variables of the equipment;
- Reducing time for start – up operations and probability of failures [8-9].

The authors have already used the HYSYS Aspen Plus software to develop the model of the reactor [10] and fractionation units [11]. The model is based on experimental data for hydrocarbon conversion on the zeolite catalysts KN –30 [12-13].

The objective of the present work is to optimize the constructive and process variables of the key equipment and operation modes.

2. Simulated process flow diagram (PFD)

PFD of gasoline conversion on zeolite catalysts is shown in Fig. 1. A feed mixture of straight – run fractions I is heated and flows to the reactor 1 with a zeolite catalyst where hydrocarbon conversion to the high – octane components of gasoline occurs.

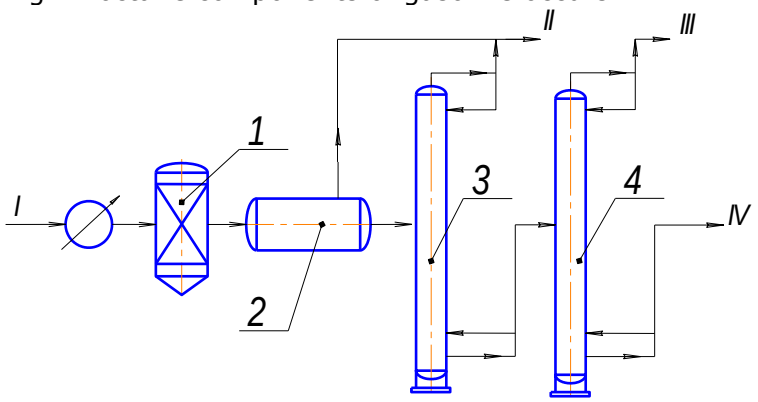

Fig. 1. PFD of gasoline conversion on zeolite catalysts: 1 – reactor; 2 – separator; 3 – stabilizing column; 4 – rectifying column; flows: I – feedstock; II – hydrocarbon gases; III – gasoline; IV – heavy residue.

Hydrocarbon gases II are partially separated from the reaction products in 2 and then serve as the process fuel. Distillation of the unstable catalizate occurs in the column 3. The bottom product of the column 3 flows to the feed section of the column 4 where the finished motor gasoline III is separated from the heavy residue IV consisting of the diesel fractions.

3. PFD Optimization

3.1. Optimal reactor design

The reaction volume of the plug flow reactor (V_p) and reaction temperature (T) were taken as the optimization variables. The objective function was developed using the product goals such as octane number and relative yield of gasoline. The tolerance intervals for the variables were taken according to the specified productivity and experimental findings: T=335 ÷ 495°C and V_p =0.6 ÷ 3.4 m^3. Fig. 2 represents the form of objective function in the space of the optimization variables.

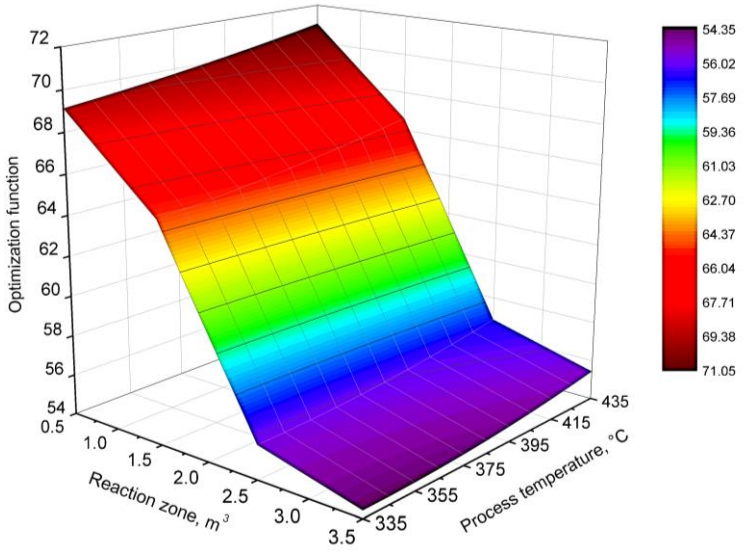

Fig. 2. The objective function.

The maximum objective function corresponds to V_p= 0.5 m^3 and T=435°C, the reactor was designed on the basis of these values (Fig. 3), and the working temperature ranges were chosen for work in the mode of maximum yield and in the mode of maximum octane number of the product.

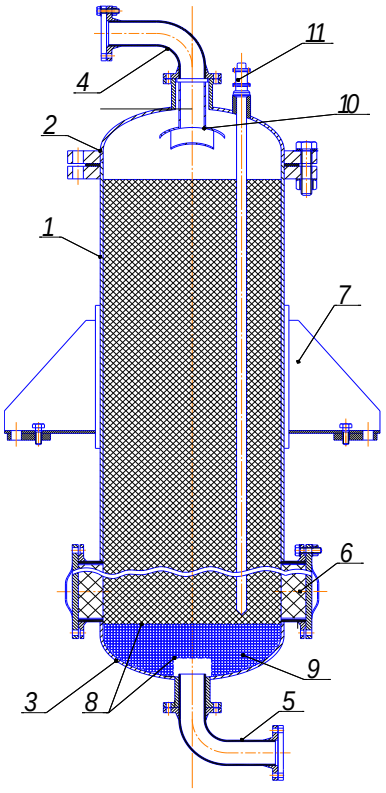

Fig. 3. Construction of the reactor:
1–reactor shell; 2–vessel lid; 3–vessel bottom; 4–inlet of feedstock; 5–outlet of products; 6–outlet for catalyst; 7–landing pad; 8–support grids; 9–porcelain balls; 10–distributor; 11–multizone thermocouples.

3.2. Optimal design of the distillation sequence

The essential requirement for distillation sequence optimization is the standard compliance of the gasoline quality [14]. The rectification profiles of temperature, pressure, and reflux rates were chosen as the optimization variables in the model. The calculation results show that pressures in the stabilizing and distillation columns significantly affect the fraction composition of gasoline.

An increase in pressure of the stabilizing column results in a change of fractional composition of the finished motor gasoline. The initial boiling point and boiling points of 10 and 50 volume percent decrease with an increase in pressure as shown in Fig. 4. An increase in pressure of the rectifying column results in a decrease in the end boiling point and point of 90 volume percent as shown in Fig. 5.

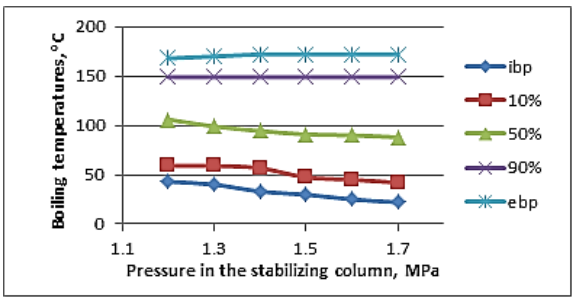

Fig. 4. Boiling temperatures (D86) vs pressure in the stabilizing column.

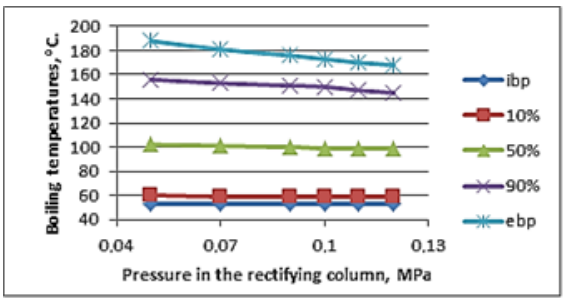

Fig. 5. Boiling temperatures (D86) vs pressure in the rectifying column.

Tab. 1 shows the results of distillation sequence optimization at various temperatures in the reactor.

Tab. 2 shows the fractional compositions (D86) of the catalyzate produced at various conversion temperatures and fractional compositions (D86) of the finished motor gasoline produced under the optimal modes of the distillation sequence. The optimal modes allow producing the gasoline that complies with the standards.

Table 1. Optimal modes for the columns

Process variable	Temperature in the reactor 395	425	445	465
Stabilizing column				
Top stage pressure, MPa	2.67	2.42	2.74	2.18
Bottom stage pressure, MPa	5.92	5.87	6.69	6.13
Top stage temperature, °C	94.1	90.7	102.1	104.2
Bottom stage temperature, °C	253.9	234.0	240.0	239.8
Rectifying column				
Top stage pressure, MPa	0.92	1.18	1.40	1.36
Bottom stage pressure, MPa	1.92	2.00	1.94	1.78
Top stage temperature, °C	219.1	212.0	206.4	219.6
Bottom stage temperature, °C	253.3	256.1	252.4	254.0

Table 2. Fractional compositions (D86) of catalyzate and finished motor gasoline

Fractional composition	GOST R 51105–97	Temperature in the reactor 395		425		445		465	
		reactor	column	reactor	column	reactor	column	reactor	column
IBP,°C	≤30	36	26.2	37	27.7	37	26.8	38	23.3
10%	≤70	64	27.8	65	33.6	76	30.5	68	25.3
50%	≤120	112	129.0	116	115.4	119	115.8	109	120.4
90%	≤180	187	144.3	171	140.6	167	139.7	145	136.0
EBP,°C	≤205	261	155.7	261	152.7	271	152.1	242	145.1

4. Conclusions

- The HYSYS Aspen Plus software was used to develop a model of the plug flow reactor and distillation sequence for products recovery.
- The developed function allows choosing optimal conditions to work in the mode of maximum yield or in the mode of maximum octane number of the finished motor gasoline.
- The optimal modes of the reactor performance were found.
- The optimal modes of the distillation sequence were found for various conversion temperatures.

Symbols

V_p - reaction volume of the plug flow reactor; T - reaction temperature.

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