As we can see from (2) and (6) criteria ε_R and ε_N are interconnected, that determines the choice of some "overall" criterion in particular

$$\varepsilon = \varepsilon_R + \varepsilon_N. \quad (7)$$

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Mathematical modeling of hydrocarbons conversion kinetics on zeolite catalysts

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The efficiency of oil refining is largely based on the use of zeolites as catalysts. The use of zeolites as catalysts in refining and petrochemistry has been considered as one of the major accomplishments in chemistry of the XXth century [1].

Zeolite catalysts have been the source of major improvements in gasoline yield and octane as well as in the production of purer fuels and lubricants with enhanced performance properties.

The following advantages make the process cost-effective and preferable for implementing:

– Low operating costs and capital investments;
– Simplicity of the technology;
– Low explosive and fire hazards due to the lack of hydrogen
– Low sensitivity of a catalyst to the quality of raw materials.

In this regard, the purpose of the work is to reduce development time of the reactor due to the pre-optimization, which will reduce time of scaling and the number of steps carried out from laboratory size to industrial scale.

This goal was accomplished by the following tasks:

At the beginning of our research we studied the mechanism of hydrocar-

bons conversion on a zeolite catalyst. The process of obtaining high-octane gasoline fractions from straight-run gasoline on zeolite catalysts includes a number of series-parallel acid-base chemical reactions occurring by a carbon-ionic mechanism. In general, the main stages of hydrocarbons conversion are presented in the scheme below:

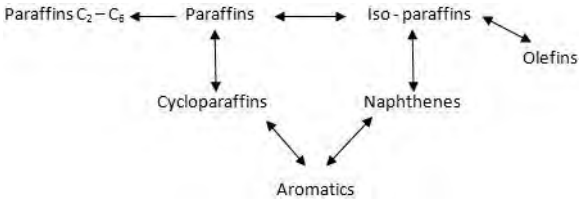

Fig. 1. *Scheme of hydrocarbons conversion on zeolite catalysts*

In the first stage of the process there typically occur reactions which lead to the cleavage of the C–C bonds of hydrocarbon, which form olefin intermediate fragments that have a high endothermic effect. In addition to these main reactions there take place other reactions such as alkylation reactions, isomerization of paraffins and naphthenes etc.

Table 1. The initial data for kinetic calculations

Reaction	K_{direct}	E_a, kDj / mole
Hexane ↔ 2-methylpentane	6	15
Hexane ↔ 3-methylpentane	6	15
2-methylpentane ↔ 3-methylpentane	6	20
2-methylpentane ↔ 2,2-dimethylbutane	3	20
3-methylpentane ↔ 2,3-dimethylbutane	3	20
2,2-dimethylbutane ↔ 2,3-dimethylbutane	6	25
Hexane ↔ Cyclohexane + H_2	6	30
2-methylpentane ↔ methylcyclopentane + H_2	3	40
3-methylpentane ↔ methylcyclopentane + H_2	3	30
Cyclohexane ↔ Benzene + H_2	3	40
Methylcyclopentane ↔ Benzene + H_2	3	40
2,3-dimethylbutane ↔ 2,3-dimethylbutene-1 + H_2	4	20
Hexane + H_2 ↔ 2 propane	0.58	16

where Kdirect, E_a – constants and activation energies of direct reactions.

Reactions model for simplified mixture was developed on the basis of experimental data. The calculation of thermodynamic characteristics for all reactions was the next stage.

We created a model of the reactor in HYSYS Aspen Tech™ using Simple Rate as a reaction model, in which reversible reactions depending on the Arrhenius equation for energy activation and equilibrium constants depending on polynomial temperature are assumed.

We took constants and activation energies for direct reactions as a first approximation on the basis of [2]. A part of initial data for kinetic calculations is shown in table 1.

The following conclusions can be made:

1. Inverse kinetic problem for hydrocarbons conversion on a zeolite catalyst has been solved;
2. Model of the reactor for the process of Zeoforming has been developed;
3. The adequacy of the model has been confirmed

Developed software for simulation and optimization allows analyzing and designing a reactor process.

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Anti-turbulent additives to oil and petroleum products

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Pipeline oil transportation is one of the most important components of Russian petrochemical complex because of the specific geography of oil fields and hydrocarbon consumption. One of the main problems in a process of oil transportation is fluid resistance. It occurs due to the resistance occurring when fluid flow meets with a solid surface, for example, pipeline wall. As a result, this fluid flow (substream) that moves to near-wall zone, spontaneously changes the direction and moves towards the center of pipeline cross