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**«НАЦИОНАЛЬНЫЙ ИССЛЕДОВАТЕЛЬСКИЙ
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ООО «СИБУР»

ХИМИЯ И ХИМИЧЕСКАЯ ТЕХНОЛОГИЯ В XXI ВЕКЕ

Материалы

XVII Международной научно-практической конференции
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Химия и химическая технология в XXI веке : материалы X46 XVII Международной научно-практической конференции студентов и молодых ученых имени профессора Л.П. Кулёва, посвященной 120-летию Томского политехнического университета (г. Томск, 17–20 мая 2016 г.) / Томский политехнический университет. – Томск : Изд-во Томского политехнического университета, 2016. – 643 с.

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В сборнике представлены материалы XVII Международной научно-практической конференции студентов и молодых ученых «Химия и химическая технология в XXI веке» имени профессора Л.П. Кулёва, посвященной 120-летию со дня основания Томского политехнического университета. В докладах обсуждаются проблемы химии и химической технологии современных органических и неорганических материалов. Большое внимание уделено физико-химическим методам анализа и их применению в исследовании лекарственных форм, объектов окружающей среды. Описаны различные ресурсосберегающие и безотходные технологии, моделирующие системы для химических процессов.

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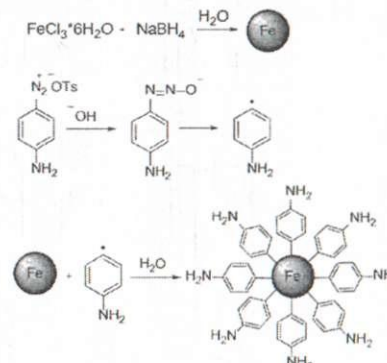
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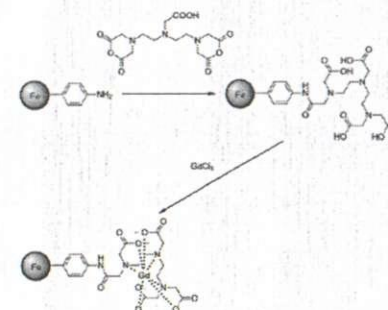
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Scheme 1. Synthesis of ZVI NPs using *p*-aminobenzenediazonium tosylate

base. Gadolinium (Gd) was chosen as a main contrast agent due to its excellent magnetic properties [3] and ability to form chelates. It was agreed to use diethylenetriaminepentaacetic acid (DTPA) anhydride to form a strong chelate with Gd because it is fairly easy attached to a free amine group of



Scheme 2. Synthesis of Gd-based MRI contrast compound

the ADS. The scheme of a process is shown in Scheme 2.

Such substance could become a base for developing new theranostic agent and further research in utilization of ZVI NPs in medical and pharmaceutical fields.

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THE TESTING OF A KINETIC MODEL OF CATALYTIC CRACKING IN THE "C-200" SECTION OF THE KT-1/1 INSTALLATION OF OIL REFINING PLANTS IN KAZAKHSTAN

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The Strategy of the development of the Republic of Kazakhstan until 2030 emphasizes the oil and gas industry, making energy resources a number one priority. This program is the basis for improving the competitiveness of the oil and gas industry of Kazakhstan [1].

Nowadays the Republic of Kazakhstan has

three oil refineries – the Atyrau Refinery, the Shymkent Refinery and the Pavlodar refinery, for which the increase in the depth of crude oil refining is an urgent task.

The aim of this work is to test the kinetic model of the process of catalytic cracking in the Section "C-200" of the installation KT-1/1 of the Pavlodar

Table 1. Group composition of vacuum distillate

The group of hydrocarbons	The vacuum distillate, the content of wt%
Paraffins + naphthenes	73.13
Aromatic hydrocarbons	23.31
Alcohol-benzene resin	3.56

reactions are presented in table 2.

The adequacy of the model calculations is presented in table 3. The adequacy of the model calculations was verified by comparing the calculated and experimental data on the concentration of the streams of hydrocarbon groups after the reactor and the gasoline fractioning.

Table 2. Kinetic parameters for catalytic cracking reactions at $T^{\circ}\text{C}=522.52$, $P=0.09$ MPa

Reactions	The rate constant		
	k_{sp}	k_{oc}	
The cracking of paraffins $\text{C}_{13}\text{-C}_{40}$	0.10	–	sec^{-1}
The cracking of isoparaffins $\text{C}_{13}\text{-C}_{40}$	0.67	–	sec^{-1}
The cracking of n-paraffins $\text{C}_5\text{-C}_{11}$	0.17	–	sec^{-1}
The isomerization of paraffins $\text{C}_5\text{-C}_{11}$	$5 \cdot 10^{-4}$	$3 \cdot 10^{-4}$	sec^{-1}
The cracking of isoparaffins $\text{C}_5\text{-C}_{11}$	0.16	–	sec^{-1}
The cracking of olefins $\text{C}_5\text{-C}_{11}$	0.67	$9.3 \cdot 10^2$	sec^{-1}
The redistribution of hydrogen	56.05	–	$1 \cdot \text{sec}^{-1} \cdot \text{mol}^{-1}$
The dealkylation of naphthenes	0.22	0	sec^{-1}
The dealkylation of aromatic hydrocarbons	0.44	$3.7 \cdot 10^{-5}$	sec^{-1}
The cracking of naphthenes	0.44	–	sec^{-1}
The condensation of aromatic compounds	2.15	–	$1 \cdot \text{sec}^{-1} \cdot \text{mol}^{-1}$
The formation of coke (polycondensation)	0.62	–	$1 \cdot \text{sec}^{-1} \cdot \text{mol}^{-1}$
The cyclization of olefins	0.05	0.016	sec^{-1}
The dealkylation of aromatic hydrocarbons of gasoline	0.15	$1.3 \cdot 10^{-5}$	sec^{-1}

Table 3. The adequacy of model calculations

Component	The calcul. wt %	Experiment, % wt.	Accuracy (relative), %
High molecular weight paraffins	3.16	3.17	0.35
Medium molecular paraffins	1.58	1.52	4.01
Isoparaffins	11.73	11.91	1.55
Olefins	7.13	7.07	0.82
Gas	33.44	33.50	0.18
Naphthenes	4.16	4.09	1.72
Monoaromatic hydrocarbons	18.66	18.68	0.13
High molecular weight naphthenes	2.36	2.33	1.40
Aromatic hydrocarbons	12.26	12.24	0.16
Gums	0.43	0.41	4.11
Coke	5.08	5.07	0.20

oil refining plant in Kazakhstan.

The testing of the kinetic model of the catalytic cracking process requires some information about the group composition of the raw materials and the catalytic cracking products. The laboratory studies were carried out to determine the group composition of the catalytic cracking products.

The kinetic parameters of the catalytic cracking

The table shows that the reactions of paraffins cracking (0.10^{-1}), hydrogen redistribution ($56.05 \text{ l} \cdot \text{s}^{-1} \cdot \text{mol}^{-1}$), the dealkylation of aromatic hydrocarbons (0.44^{-1}) and naphthenes (0.22^{-1}), as well as the condensation of aromatic compounds ($2.15 \text{ l} \cdot \text{s}^{-1} \cdot \text{mol}^{-1}$) and the coke formation ($0.62 \text{ l} \cdot \text{s}^{-1} \cdot \text{mol}^{-1}$) occur at the greatest speed.

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THE IMPACT OF CATALYST TEMPERATURE FROM REGENERATOR ON THE CATALYTIC CRACKING PROCESS PERFORMANCE

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The yield and composition of the catalytic cracking products are determined by a whole set of records of operation for non-stationary adjoin system "riser-regenerator".

The most important parameters of a technological mode determined by the temperature of the catalytic cracking process are the catalyst temperature after regeneration, feedstock temperature, the ratio of catalyst: feedstock and steam flow into the

reaction zone of the riser reactor [1]. Catalyst circulation ratio is determined depending on the temperature of the catalyst after regeneration, which in turn depends on the coke content on the catalyst after the riser reactor. Coke content depends from the composition of the feedstock and temperature mode of the riser reactor.

The purpose of this research is to evaluate the effect of catalyst temperature on the vacuum distil-

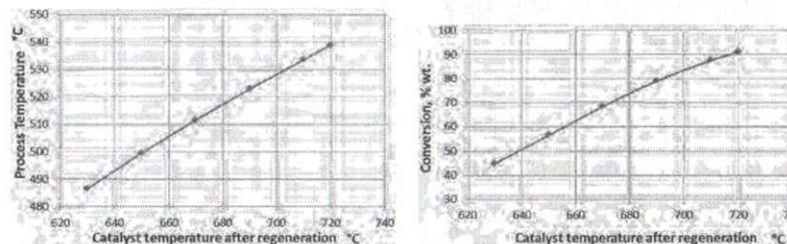


Fig. 1. The impact of catalyst temperature after regeneration on the process temperature and on the conversion of feedstock

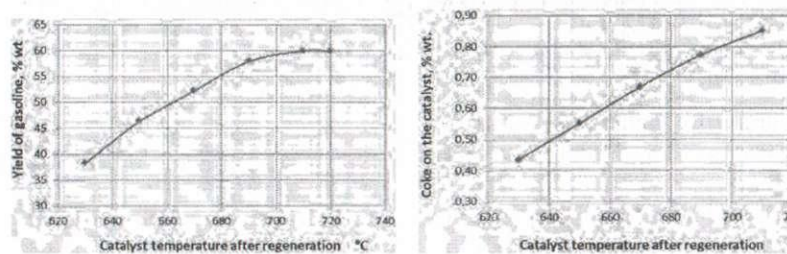


Fig. 2. The impact of catalyst temperature after regeneration on the gasoline yield and on the coke content on the catalyst

late conversion and coke content on the catalyst in the catalytic cracking.

Calculations of the temperature effect of regenerated catalyst on the catalytic cracking performance carried out using by mathematical model of the catalytic cracking [2]. Catalyst temperature after regeneration stage varied in the range of (630–720) °C.

The process temperature increases from 486 to 539 °C and the degree of conversion of the catalytic cracking feedstock increases from 44 to 90% wt. (fig. 1) with increasing the temperature of regenerated catalyst in the range of 630–720 °C. In this case initially increases gasoline yield (to the temperature of regenerated catalyst 710 °C), then observed the decrease of gasoline yield (is a "re-cracking" process) and increasing of gas product yield from 4.05 % wt. (process temperature 486 °C) to 25.6 % wt. (at 539 °C). The maximum theoretical yield of gasoline

is 59.9 % wt. However, the rate of coke formation reactions and the content of coke on the catalyst increases from 0.44 to 0.88% by weight.

Thus, the products yield from the catalytic cracking unit depends largely on the temperature of regenerated catalyst. Increasing the catalyst temperature after regenerator from 630 to 720 °C at a constant ratio of catalyst:feedstock 5.56 provides the increase of process temperature from 486 to 539 °C, the degree of conversion increase more than 40% and coke content on the catalyst at 0.44% wt. In this case, the gasoline fraction yield passes through a maximum (59.9 % wt.). The optimization of process conditions depending on the temperature of the regenerated catalyst and the feedstock composition is important to obtain the maximum yield of gasoline fraction and a low content of coke on the catalyst.

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EFFECT OF RADIATION ON CHARACTERISTICS OF EPOXY POLYMER

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Today, many fields of human activity can produce radioactive wastes. Because of the nature of this kind of waste, it needs proper management and treatment methods in order to protect human health and environment, not only for current time, but also in the future generation.

There are many ways to immobilize radioactive wastes, they depends on the nature of the wastes (its radioactivity, forms), final disposal facility conditions, technology and budget available [1]. In general, based on the matrix materials, we can divide radioactive waste mobilization methods to several groups:

- Cementation: cement is an inorganic material that has the ability to react with water at ambient conditions to form a hardened mass. Cement are usually utilized to conditioning

large amount of low level radioactive waste because its availability and reasonable cost. However, cementation is poorly incorporated with organic-based liquid wastes.

- Bituminization: bitumen is a thermoplastic material and contains a mixture of high molecular weight, which obtained as a residue in petroleum or coal tar refining. Unlike cement, bitumen could be used to immobilize organic wastes such as waste oil. As a high molecular hydrocarbon, bitumen is expected to withstand well against environmental conditions.
- Vitrification: this method designed to immobilize waste for a long time in compact solid, insoluble form by combining solid waste with glass-forming material like borosilicates, and then heating the mixture under high

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