

**Раздел 5. «Химия»**

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(E-mail: r.zhaslan@ttu.edu.kz)**Study on the influence of iron particle size on primary coal tar**

This study aims to investigate how iron particle size affects fraction yield at different temperatures (up to 200°C and 200-300°C) in catalytic hydrodynamic and hydrogenation processes of primary coal tar. Various sizes of iron particles were added to the resin and processed at different temperatures. After analyzing the obtained products, it was found that the size of iron particles affects the yield of the fraction under various processing conditions. The data obtained allow us to conclude that the average particle size of nanocatalyst iron particles in the range from 10 to 50 nm has a positive effect on the yield of light and medium fractions from primary hydrogenation product. coal tar and the individual chemical composition of the above-mentioned fractions. The results obtained can be used to optimize coal tar processing processes in industry.

*Key words:* iron, coal tar, nanocatalysts, resin, chemical synthesis, fuel hydrogenation, fraction, hydrogenation.

*Introduction*

The study of the effect of iron particle size on the fraction yield during catalytic hydrodynamic and hydrogenation processing of primary coal tar is relevant in the context of the search for effective and environmentally friendly methods for processing hydrocarbon raw materials. Given the growing interest in the use of hydrocarbons in fuel production, chemical industry and other industries, optimization of coal tar processing processes has become an important task [ 1-3 ].

From literary sources [4,5] it is known that nanocatalysts are more effective in the process of hydrogenation of solid and heavy hydrocarbon feedstocks compared to known catalysts. The authors of [4] found that the particle sizes of nanocatalysts affect the activity and selectivity in the process of hydrogenation of model organic compounds.

*Methods and materials*

To find the optimal average size of iron particles, nanocatalysts for the yield of fractions up to 200°C and 200-300°C during the hydrodynamic action of primary coal tar were carried out on a laboratory installation GDN-1, and the hydrogenation of primary coal tar was carried out under autoclave conditions. Screenings of nanocatalysts  $\beta$ -FeOOH and Fe<sub>3</sub>O<sub>4</sub> were carried out using sieves and the following fractions were selected: 0-0,075 mm; 0-0,1 mm; 0-0,15 mm and 0-0,2 mm. The average particle diameter sizes of the selected fractions of nanocatalysts were determined in water using a laser particle size detector. The average size of iron particles in  $\beta$ -FeOOH and Fe<sub>3</sub>O<sub>4</sub> nanocatalysts for the selected ones was: 10 nm (0,075 mm), 25 nm (0,1 mm), 30 nm (0,15 mm) and 50 nm ( 0,2 mm).

*Results and discussion*

It has been established that the nature of the change in the yield of the fraction up to 200°C and 200-300°C during the catalytic-hydrodynamic effect on primary coal tar is symbiotic for the  $\beta$  FeOOH and Fe<sub>3</sub>O<sub>4</sub> nanocatalysts. Preliminary experiments on the hydrogenation of the light fraction of primary coal tar showed that the average particle size of the Fe<sub>3</sub>O<sub>4</sub> nanocatalysts does not have a significant effect on the yield of the light and medium fraction from the hydrogenate. Only the  $\beta$ -FeOOH nanocatalyst was used in the experiments. When the average particle size changes from 10 to 25 nm, the highest yield of the light fraction is observed from 6.5 to 17.6%, and the yield of the middle fraction from primary coal tar similarly increases from 16 to

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17.6% during the hydrodynamic effect on primary coal tar. With an increase in the average size of iron particles, the yield of the fraction from the hydrogenated product changes extremely: with an average size of iron particles of 25 nm for the yield of the light and medium fractions, a local maximum appears (Table 1), the lowest fraction yield is observed in the range from 30 to 50 nm.

Table 1 - Effect of the average particle size of the nanocatalyst  $\beta$  FeOOH on the yield of light and medium fractions from the hydrogenation of primary coal tar (hydrodynamic heating).

№	Average particle size of iron nanocatalyst $\beta$ FeOOH, nm	Yield of light and medium fractions from primary coal tar hydrogenation product, wt %	
		up to 200 <sup>0</sup> C	200-300 <sup>0</sup> C
1	Without catalyst	2.5	13.0
2	10	6.5	16.0
3	25	12.6	17.6
4	30	7.4	16.0
5	50	5.2	14.4

The results presented in Table 1 on the catalytic-hydrodynamic effect showed that the average particle size of the iron nanocatalyst affects not only the yield of light and medium fractions from the hydrogenation product, but also the qualitative and quantitative composition of the resulting liquid products. Figures 1-2 show chromatograms of the light and medium fractions obtained from the hydrogenation of primary coal tar. As can be seen from the data presented in figure 1 and table 1, the average size of iron particles affects the distribution of paraffin and aromatic hydrocarbons and phenols and phenol-containing substances. It should be noted that in the light fraction the content of aromatic hydrocarbons (benzene, o.xylene, methyl-1-propylbenzene, etc.) increases quite significantly from 0.5 to 4.7%, with an increase in the average size of iron particles from 10 to 30 nm. The amount of paraffin hydrocarbons similarly increases from 0.2 to 5.7%, the concentration of phenols does not decrease significantly from 18.1 to 17.2. In the 200-300<sup>0</sup>C fraction, the concentration of aromatic and paraffin hydrocarbons similarly increases, depending on the average size of the nanocatalyst iron particles. In addition, the content of decane and dodecane increases from 0.2 to 1.1 and 0.1 to 1.5%, respectively.

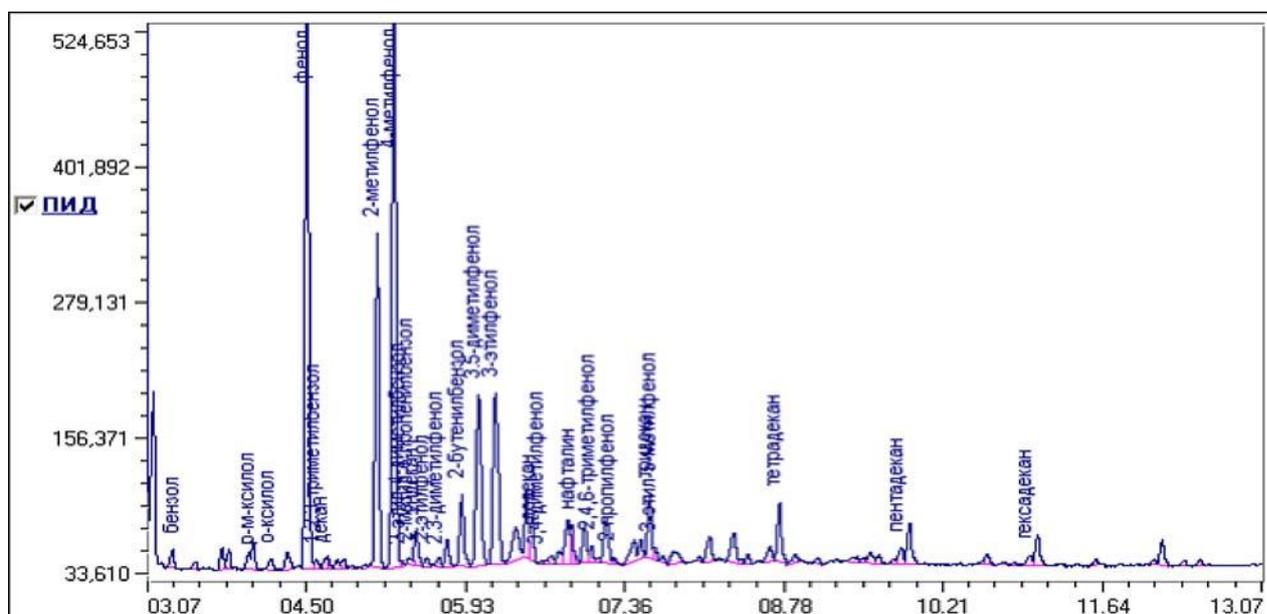


Figure 1 - Chromatogram of the fraction up to 200<sup>0</sup>C (average iron particle size 25 nm)

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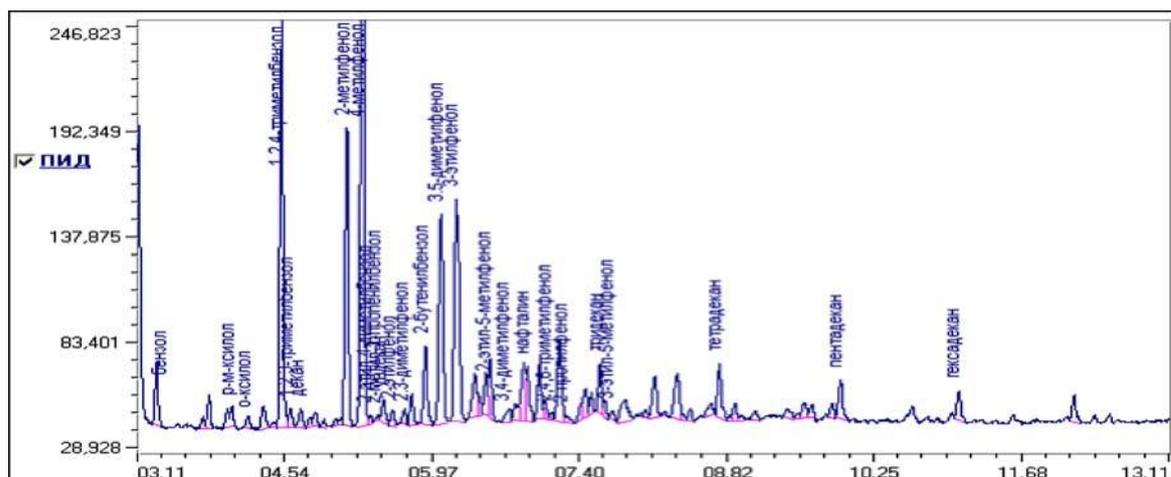
Figure 2 - Chromatogram of the fraction 200 - 300<sup>0</sup>C (average iron particle size 25 nm)

Table 2 shows the effect of the average particle diameter of the nanocatalyst on the yield of the fraction up to 200 <sup>0</sup>C and 200-300 <sup>0</sup>C. With an increase in the average size of the nanocatalyst particle diameter in the range from 10 to 50 nm, the yield of the light and medium fraction from the hydrogenation product increases from 5 to 17.4% (fraction up to 200 <sup>0</sup>C) and from 19.2 to 37.4% (fraction up to 200-300 <sup>0</sup>C).

Table 2 - Effect of the average particle size of the nanocatalyst  $\beta$ -FeOOH on the yield of light and medium fractions from the hydrogenation product during the hydrogenation of PCT.

№	Average particle size of iron nanocatalyst $\beta$ FeOOH, nm	Yield of light and medium fractions from PCT hydrogenate, wt %	
		up to 200 <sup>0</sup> C	200-300 <sup>0</sup> C
1	Without catalyst	5.0	19.2
2	10	8.5	23.4
3	25	15.7	35.1
4	30	16.2	36.2
5	50	17.4	37.4

The experimental results shown in table 2 in comparison with experiments without catalysts proceed with a low yield of light and medium fractions of almost 1.5-2 times, and the yield of gaseous and solid products increases by 2-2.5 times.

With the average particle size of nanocatalysts  $\beta$ -FeOOH and Fe<sub>3</sub>O<sub>4</sub> under the conditions of hydrogenation of primary coal tar, it selectively hydrogenates polyaromatic compounds of primary coal tar (anthracene, phenanthrene, biphenyl, acenaphthene, etc.) with subsequent destruction of products into low molecular weight compounds and thereby increasing the yield of light and the middle fraction from the hydrogenation of primary coal tar.

### Conclusions

The results obtained indicate that, under hydrodynamic influence on primary coal tar, the average size of nanocatalyst iron particles influences the deep decomposition of primary coal tar molecules with the rapid occurrence of a variety of reactions: dealkylation, hydrogenation, isomerization, etc. As a result of these reactions, the formation of free radicals that interact with each other, but ultimately produce hydrocarbons of lower molecular weight in the system.

Thus, the data obtained allow us to conclude that the average particle size of nanocatalyst iron particles in the range from 10 to 50 nm has a positive effect on the yield of light and medium fractions from the

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hydrogenation of primary coal tar and on the individual chemical composition of the above-mentioned fractions.

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**Бастапқы көмір шайырына темір бөлшектерінің мөлшерінің әсерін зерттеу**

Бұл зерттеу жұмысы темір бөлшектерінің мөлшері бастапқы көмір шайырының каталитикалық гидродинамикалық және гидрогенизациялық өңдеу процестерінде әртүрлі температурада (200°C және 200-300°C дейін) фракцияның шығуына қалай әсер ететінін зерттеуге бағытталған. Шайырға темір бөлшектерінің әртүрлі өлшемдері қосылды және әртүрлі температурада өңделді. Алынған өнімдерді талдағаннан кейін темір бөлшектерінің мөлшері әр түрлі өңдеу жағдайында фракцияның шығуына әсер ететіндігі анықталды. Нәтижелер 10-нан 50 нм аралығындағы нанокатализатор темір бөлшектерінің орташа мөлшерінің жеңіл және орташа фракцияның бастапқы көмір шайырының гидрогенизатынан шығуына және жоғарыда аталғандардан жоғары жеке химиялық құрамға оң әсері туралы қорытынды жасауға мүмкіндік береді. Фракциялар. Алынған нәтижелер өнеркәсіптегі көмір шайырын өңдеу процестерін оңтайландыру үшін пайдаланылуы мүмкін.

*Түйін сөздер:* темір, көмір шайыры, нанокатализаторлар, шайыр, химиялық синтез, отынды гидрлеу, фракция, гидрогенизация.

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**Исследование влияния размерности частиц железа на первичную каменноугольную смолу**

Данное исследование направлено на изучение того, как размер частиц железа влияет на выход фракции при различных температурах (до 200°C и 200-300°C) в процессах каталитической гидродинамической и гидрогенизационной обработки первичной каменноугольной смолы. Различные размеры частиц железа были добавлены к смоле и подвергнуты обработке при различных температурах. После анализа полученных продуктов было установлено, что размер частиц железа оказывает влияние на выход фракции при различных условиях обработки. Полученные данные позволяют сделать вывод о положительном влиянии величины среднего размера частиц железа нанокатализатора в интервале от 10 до 50 нм на выход легкой и средней фракции из

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гидрогенизата первичной каменноугольной смолы и на индивидуальный химический состав выше названных фракции. Полученные результаты могут быть использованы для оптимизации процессов обработки каменноугольной смолы в промышленности.

*Ключевые слова:* железо, каменноугольная смола, нанокатализаторы, смола, химический синтез, гидрирование топлива, фракция, гидрогенизация.

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