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Contents

the emergency well with the emergency object, i.e. fibreglass rod. According to the specified design of the rod-header (Fig.2), its main gripping element is the spiral and collet parts located in the tool body. The end of the body or coupling of the fibreglass rod, when lowering the rod head, goes through the funnel inside the body of the rod head and the internal surface with notches of the gripping elements of the spiral and collet of this rod is captured. It is covered with its inner surface with notched gripping elements, over the entire diameter of the end of the body or coupling of the fibreglass rod. The body of the glass fibre rod has a smoother surface compared to metal, steel rods. Consequently, the possibility of accident elimination, i.e. extraction of the emergency object of the glass fibre rod from the well depends on the reliable process of engagement of the smooth surface of the end of the body or coupling of this rod with notches of the inner surface of the gripping elements, i.e. spiral and collet. That is to say, having a high coefficient of friction between these surfaces, the possibility of retrieving the fibreglass rod remaining in the borehole is more likely. Fixation and compressive force, i.e. from the large elastic properties of these gripping elements also makes it likely that the smooth surface of the body or end of the coupling of the fibreglass rod can be grasped and extracted from the well. Engagement of the gripping elements by their internal surface with notches along the entire diameter of the coupling end or body of the fibreglass rod indicates the factor of technological fit between these surfaces. The tight fit formed between these surfaces makes it possible to eliminate the accident with fibreglass rods with the help of a rod-header designed for them.

Conflict of interest

The authors declare that they have no conflict of interest in relation to this research

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Modeling and optimization of the process hydrotreating of diesel fuel

N.M.Abbasov*, A.A. Məsimov

* Research Institute of Geotechnologocal Problems of Oil, Gas and Chemistry, ASOIU, 20 Azadlig Ave., Baku, AZ-1010 Azerbaijan
Department of Industrial machines, ASOIU, 20 Azadlig Avenue. AZ-1010 Azerbaijan

Abstract

The main approaches to the development of a reactor unit for the hydro desulfurization of diesel fuels are considered, taking into account the reactivity of the organosulfur components that make up diesel fuel and the formation of pseudocomponents conditionally combining a group of organosulfur components. As the concentration of easily or difficult-to-hydrogenate sulfur-containing components in raw materials increases, the role of a substance limiting the quality of diesel fuel purification may shift from an easily hydrogenated to a difficult-to-hydrogenate

pseudocomponent and vice versa. The efficiency of operation of five variants of the reactor unit of hydrotreating plants is compared. It is shown that from the point of view of minimizing the loading of the catalyst, the two-reactor scheme of the hydrotreating process with separate supply of low-boiling and high-boiling fractions of straight-run diesel fuel to the reactors is optimal. The necessity of determining the temperature boundary of their division, taking into account the qualitative and quantitative composition of these fractions by organosulfur substances, is substantiated.
Keywords: hydrotreating, diesel fuel, mathematical modeling and optimization of hydrotreating, kinetics of chemical reaction, organosulfur substances
*Corresponding author. Tel.: + 994 506139897
E-mail:

1. Introduction

Hydrotreating of diesel fuel is one of the largest-tonnage petrochemical processes. The specificity of the process lies in the fact that its implementation is carried out in the presence of a number of adverse factors [1]. These include:

– carrying out the process at very high pressures of 3-8 MPa;

– low content of organosulfur compounds in the feedstock – 1.5–0.8 wt. %, as a result of which hydrotreating as a chemical process occurs at very low rates of desulfurization reaction;

– the process as a whole is carried out in the most difficult to implement three-phase system: liquid-phase raw materials, hydrogen-containing gas, bifunctional solid catalysts that ensure the implementation of homolytic and heterocyclic reactions [2, 3];

– a large number of various organophosphorus compounds, which significantly complicates the formation of mathematical models of the process;

– simultaneously with hydro desulfurization, a large number of additional reactions involving hydrogen (hydrodeazotization, hydronitration of aromatic hydrocarbons) occur;

– strict requirements for the quality of diesel fuel, limiting the sulfur content;

– gradual deactivation of the catalyst, which leads to instability of the operation of hydrotreating plants.

While low requirements for the quality of diesel fuel were ensured by reducing the total sulfur content as a result of hydrotreating by 5-10 times, it did not matter that different organosulfur components of raw materials have different hydrogenation rates.

This made it possible to use in calculations a quasi-homogeneous scheme of the desulfurization process as a whole [4, 5] according to the scheme of the generalized reaction:

$$RS + H_2 \rightarrow HC + H_2S,$$

where RS, H_2, HC, H_2S are, respectively, the total organosulfur substance, hydrogen, hydrocarbon, hydrogen sulfide.

In this case, due to the fact that hydrogen is introduced into the hydrotreating process in large excess (consumption of hydrogen-containing gas 200-800 m^3/m^3 of raw materials), the desulfurization reaction could be considered as a pseudo-first-order reaction and the kinetics of hydrotreating was described by the equation:

$$\frac{dC_{RS}}{d\tau} = -KC_{RS},$$

where C_{RS} is the concentration of a generalized set of organosulfur components in the reaction system, τ is the reaction time, and K is the reaction rate constant, which, due to accepted assumptions, is effective

As the requirements for the quality of diesel fuel became stricter and the level of permissible sulfur content decreased by standards from Euro-3 (350 million^{-1}) to Euro-5 (10 million^{-1}), the schemes of reactor units of the hydrotreating plant began to improve with the transition from single reactors to more complex systems: two-reactor schemes with series and parallel reactors, three-reactor schemes, reactors with several layers of catalysts of different selectivity, the use of a recycle of purified raw materials, etc. [6-14].

At the same time, they began to delve into mathematical models of hydrotreating.

The degree of activity of sulfur compounds in hydrogenolysis reactions varies and decreases in the series: mercaptans > sulfides > thiophenes > benzothiophenes > dibenzothiophenes. At the same time, the most difficult-to-hydrogenate compounds of the thiophene series are concentrated mainly in heavy fractions boiling above 330°C. With an increase in the temperature of the process, the degree of hydrogenation of sulfurous and unsaturated the dehydrogenation of naphthenes increases, however, at values above 420°C, the effectiveness of the target reactions decreases markedly due to the transition of the process to the diffusion zone, but the rate of cracking reactions increases, provoking the formation of coke, and the catalyst itself begins to sinter with the destruction of the porous structure. Therefore, the main attention is paid to the formation of mathematical models of hydrogenation kinetics in the temperature range 320-380°C [15-20] with alternative approaches to solving the problem. The first approach is to identify an extremely complete set of organosulfur components of diesel fuel and develop a database of possible reaction routes, for example, [21] describes 38 hydrogenation reactions of organosulfur components with the number of carbon atoms in a molecule from 2 to 12, belonging to the following groups of substances: mercaptans, sulfides, disulfides, thiophenes, benzothiophenes, dibenzothiophenes.

However, it is quite problematic to implement kinetic experiments to obtain the physicochemical characteristics of reactions necessary for modeling the process, primarily the constants of the Arrhenius equation (activation energy and preexponential multiplier) due to the microconcentrations of many components in the reaction mixture.

The second approach consists to a certain extent in formally combining the components of one group of organosulfur substances into a conditional pseudocomponent, but at the same time the calculated constants of both the Arrhenius equation and the reaction rate constants themselves are effective and do not allow an objective analysis of the reaction process to be formed. For example, in [15], the study of the desulfurization process of diesel fuel was performed using the following conditional pseudocomponents: combined sulfides, combined ethylbene-zothiophenes, combined propylbenzothiophenes, combined butylbenzothiophenes, dibenzothiophene, combined methyldibenzothiophenes and combined ethyldibenzothiophenes, and in [22]

A different grouping was used: combined aliphatic and non-heterocyclic sulfurcontaining components, including thiols, sulfeeds and thiophenes, benzothiophene, combined benzothiophenes, including alkyl chains from 1 to 5 carbon atoms, dibenzothiophene, combined dibenzothiophenes, including alkyl chains from 1 to 5 carbon atoms, while in the course of mathematical modeling of hydrotreating, far from equivalent compositions of raw materials are taken into account, including organosulfur components (Table 1).

From the standpoint of the direct use of mathematical models for the control of industrial hydrotreating reactors, more The second direction is rational, however, a detailed analysis of the process is necessary, taking into account the organosulphurization components that limit the depth of hydrodesulfurization of diesel fuel.

2. Methodological part

It is obvious that ensuring the depth of purification of diesel fuel to the required permissible level of sulfur content is determined not by the total content of organosulfur components in the fuel being cleaned, but by a combination of two factors: the concentration and reactivity of the most characteristic impurities [21-23] combined into pseudocomponents. An increase in the concentration of any pseudocomponent leads to an increase in the duration of hydrotreating and, accordingly, a proportional increase in the loading of the catalyst into the reactor. Availability in raw materials hydrotreating of a hard-to-hydrogenate pseudo-component also leads to an increase in the duration of hydrotreating and an increase in the loading of the catalyst into the reactor.

Figure 1 shows variants of generalized schemes of the chemistry of the hydrotreating process with a different number of conditional pseudocomponents.

Table 1. The content of pseudocomponents in diesel fuels

Pseudocomponent		The proportion of the pseudocomponent in organosulfur substances, wt. %	
		according to [15]	according to [22]
Combined aliphatic and heterocyclic sulfur-containing components, thiols, sulfides, thiophenes		-	3.2
Benzothiophene		-	11.5
Combined methylbenzothiophene		-	14.1
Combined ethylbenzothiophenes		21.5	17.9
Combined propylbenzothiophene		34.8	20.5
Combined butylbenzothiophene		33.2	23.2
Combined pentylbenzothiophenes		-	
Dibenzothiophene		7.9	2.6
Combined methyldibenzothiophene		2.4	6.4
Combined ethyldibenzothiophenes		0.1	

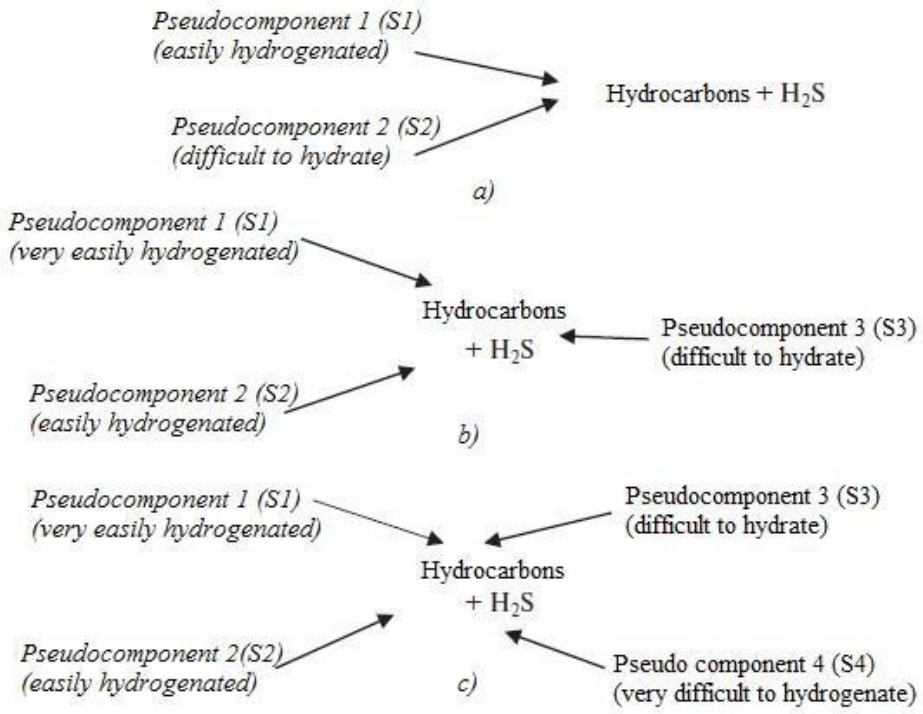

Fig. 1. Generalized schemes of the hydrotreating process with the number of pseudo-components two (a), three (b) and four (c) according to [22].

The model of the kinetics of the hydrotreating process, for example, for four pseudo-components has the form of a system of equations:

$$\left.\begin{aligned}\frac{dC_{S1}}{d\tau} &= -K_1 C_{S1}\\ \frac{dC_{S2}}{d\tau} &= -K_2 C_{S2}\\ \frac{dC_{S3}}{d\tau} &= -K_3 C_{S3}\\ \frac{dC_{S4}}{d\tau} &= -K_4 C_{S4}\end{aligned}\right\}$$

$$C_{RS} = C_{S1} + C_{S2} + C_{S3} + C_{S4},$$

where C_{Si} and K_i are, respectively, the concentration of the organosulfur pseudocomponent and the rate constant of the i–th reaction

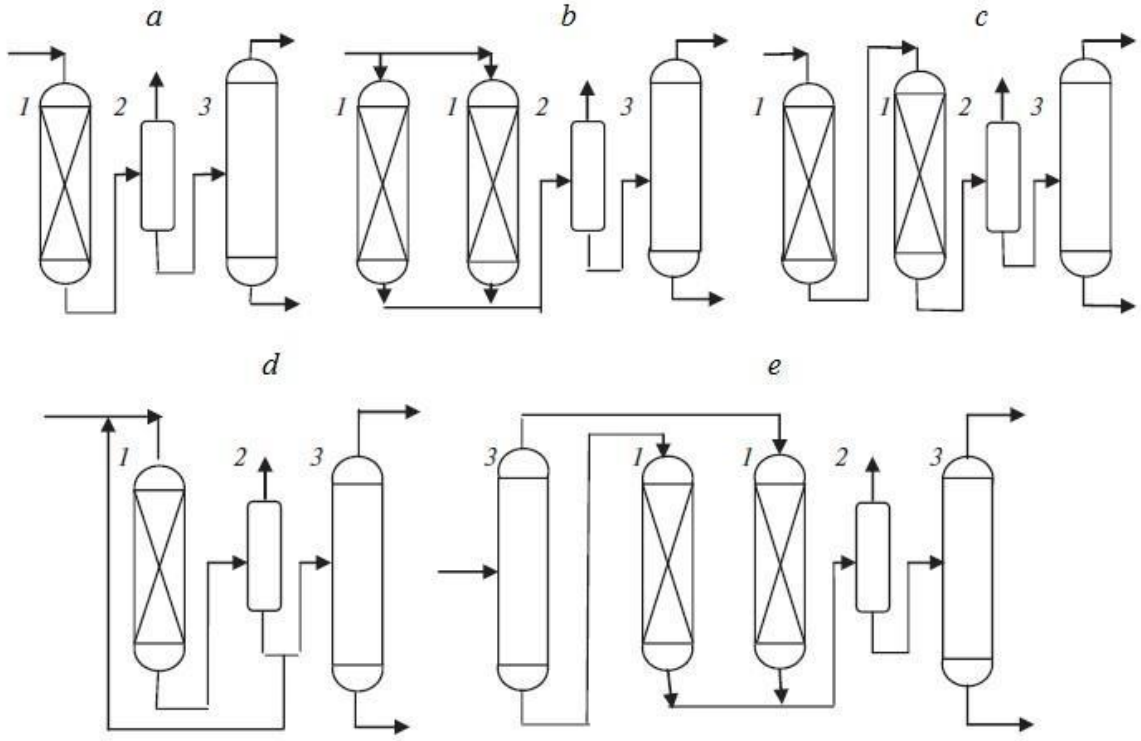

Fig. 2. Schematic diagrams of reactor units: (a) – single–reactor unit [24], (b) – two–reactor unit with parallel feed of raw materials [25], (c) – two-reactor unit with sequential feed of raw materials [25, 26], (d) – single-reactor unit with recirculation of purified diesel fuel [27], (e) – a two–reactor unit with preliminary fractionation of raw materials [28]; 1 – reactor, 2 – separator, 3 – distillation column.

The variety of hardware design of the reactor unit of hydrotreating plants (Fig. 2) requires a fairly detailed analysis from the standpoint of minimizing the loading of the catalyst to obtain high-quality diesel fuel. Since the reactors are structurally the same in all circuits, when solving the task, it was assumed that the ideal displacement regime is implemented in the reactors from the standpoint of hydrodynamics and isothermicity of the process was assumed to simplify calculations, since with constant depth of hydrotreating and other things being equal, the temperature profile in the height of the catalyst layer in reactors of different circuits should be almost the same.

To compare different reactor systems of hydrotreating stem (Fig. 2), mathematical modeling of the hydrodesulfurization process of 250 m^3/h of diesel fuel with a sulfur content of 6000 mg/kg (6000 mln^{-1}) was performed at a volumetric feed rate of 2 h^{-1} and the accepted effective rate constant of the hydrodesulfurization reaction of 2 h^{-1} [15], that, with constant technological parameters (temperature, pressure, flow rate of hydrogen-containing gas), it was possible to correctly consider a rather complex catalytic hydrotreating process as a quasi-homogeneous reaction of the first order. Calculations the differential equations of the model were performed by the Runge–Kutta method with the determination of the required contact time of the reaction mixture with the catalyst. The efficiency of the reaction system in ensuring the final concentration of sulfur in purified diesel fuel from 500 to 10 mg/kg was estimated by the total volume of the catalyst in the

reaction system, represented by a single reactor, two parallel reactors, two sequentially operating reactors and a single a reactor with a purified diesel fraction fed into it as a recycle after separation of hydrogen-containing gas, which was supposed to shorten the duration of the reaction by reducing the sulfur concentration at the reactor inlet.

The calculations showed (Table. 2) that the volume of the catalyst in a single reactor, and in a parallel and sequential reactor system, necessary to achieve a given residual sulfur concentration in diesel fuel, is the same and the configuration of the installation scheme is determined only by technical limitations.

The supply of a recycle of purified diesel fuel from the separator to the reactor is irrational, since this technique leads to an increase in the reaction volume, all other things being equal (Fig. 3, Table. 2), since, despite a slight decrease in the duration of the hydrodesulfurization process, the actual flow rate of the cleaned stream increases significantly due to the additional recirculation contribution.

Calculation of several options for the hydrotreating process of model diesel fuel with a total sulfur content of 1000 mln^{-1}, but with different the content of easily and difficult-to–hydrogenate conditional pseudocomponents with reaction rate constants of 20 and 5 h^{-1}, respectively, showed that for a process implemented in a single reactor, as the concentration of difficult-to-hydrogenate sulfur-containing pseudocomponents in raw materials increases, the role of limiting the quality of diesel fuel purification gradually shifts from an easily hydrogenated to a difficult-to-hydrogenate pseudocomponent (Fig. 4, Table 3).

To switch from the degree of hydrotreating of raw materials from 95% (residual sulfur content of 50 $million^{-1}$) to 99% (residual sulfur content of 10 $million^{-1}$), it is necessary to double the duration of the process and, accordingly, the loading of the catalyst into a single reactor (Table 2).

The greatest interest is from the standpoint of minimizing the loading of the catalyst into hydrotreating reactors The original scheme (Fig. 2,d) is presented, which was proposed in [28, 29] and considers the preliminary separation of the initial diesel fuel into light (180-300°C) and heavy (300-360°C) fractions with their separate hydrotreatment in two reactors to the required depth of hydrodesulfurization, which made it possible to increase the depth of hydrotreatment of diesel fuel at the L-24-6 RNPZ unit without changing the loading of the catalyst into the reactors [29].

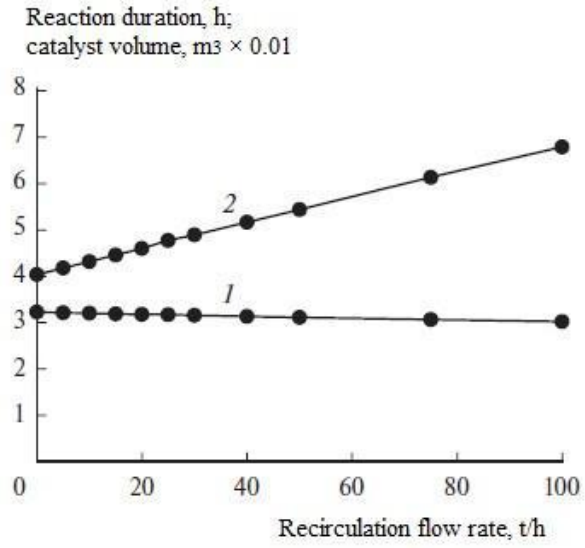

Fig. 3. Dependence of the reaction duration (1)

and the volume of the catalyst (2) on the recirculation flow rate at the residual sulfur concentration in diesel fuel 10 million^{-1}.

Table 2. Modeling of various reaction systems for hydrotreating diesel fuel

The reaction system	Recirculator flow rate, t/h	Final sulfur concentration, mg/kg	Reaction time, h	Volume of the catalyst, m^3
Diagrams of Fig. 2a, 2b, 2c – one reactor, two serial or two parallel reactors	0	2000	0.550	68.8
Diagrams of Fig. 2a, 2b, 2c Diagrams of Fig. 2a, 2b, 2c Diagrams of Fig. 2a, 2b, 2c Diagrams of Fig. 2a, 2b, 2c	0	500	1.245	155.6
Diagram fig. 2d – reactor with recirculation	10	500	1.220	164.7
Diagram fig. 2d	30	500	1.175	182.1
Diagram fig. 2d	50	500	1.130	197.7
Diagram fig. 2d	10	350	1.400	189.0
Diagram fig. 2d	30	350	1.350	209.2
Diagram fig. 2d	50	350	1.310	229.2
Diagram fig. 2d	10	50	2.370	319.9
Diagram fig. 2d	30	50	2.325	360.4
Diagram fig. 2d	50	50	2.285	399.8
Diagram fig. 2d	10	10	3.175	428.6
Diagram fig. 2d	30	10	3.130	485.1
Diagram fig. 2d	50	10	3.085	539.8

The disadvantage of this two-reactor scheme is the rigid temperature limit of 300°C separation of the initial diesel fuel into light and heavy fractions, since the efficiency and depth of hydrotreating are influenced not only by the reactivity of organosulfur substances, but also by their concentration (Table 3). For a detailed analysis of the effect of both the reactivity and concentration of organosulfur substances and the search for the optimal boundary for dividing raw materials into light and heavy fractions, mathematical modeling of the hydrotreating process of straight-run diesel fuel with boiling limits of 180-365°C, which potentially contains more than 30 organosulfur components (mercaptans, sulfides, disulfides, thiophenes) was performed by analogy with [22] were grouped in four conditional pseudocomponents contained in four narrow fractions and characterized by conditional reaction rate constants, The values of which are taken in proportion to the corresponding rates of hydrodesulfurization reactions of various classes of organosulphurization components (Table 4).

During the mathematical modeling of the hydrotreating process, the concentrations of four pseudocomponents (respectively C_1, C_2, C_3, C_4) varied and the reaction time and the required

volume of the catalyst for four variants of the process were determined, provided that the concentration of sulfur in the final hydrogenate does not exceed 10 mln^{-1}. In the first variant, all the raw materials in the amount of 100 m^3/h are supplied to one reactor, in other variants, the raw materials are pre-fractionated in a distillation column into light and heavy fractions, each of which includes specific narrow fractions and pseudo-components according to Table 5, separately entering the first and second reactors, respectively (Table 5).

In all series of calculations, a change in the volume of the catalyst loaded into the reactor was observed block, when redistributing light and heavy fractions of the initial diesel fuel over two reactors with a minimum volume at a certain temperature boundary of the separation of raw materials in the distillation column.

Table 3. The effect of the share of the hard-to-hydrogenate component Z in the total amount of sulfur-containing substances in model diesel fuel on the hydrotreatment of raw materials to the level of 95 and 99%

Parameters	Z, mass. %					
	0.20	0.15	0.10	0.07	0.05	0.03
Sulfur content in raw materials, mln^{-1}:						
– general	1000	1000	1000	1000	1000	1000
– easily hydrated	800	850	900	930	950	970
– difficult to hydrate	200	150	100	70	50	30
Sulfur content in hydrogenate, mln^{-1}:						
– general	50	50	50	50	50	50
– easily hydrated	2.54	6.19	14.43	22.43	20.09	36.76
– difficult to hydrate	47.45	43.81	35.36	27.57	20.90	13.24
The duration of the process (c) until the degree of purification is reached						
– 95% (S_{extr} = 50 $million^{-1}$)	1035	886	744	670	627	589
– 99% (S_{extr} = 10 $million^{-1}$)	2200	1950	1600	1400	1200	100

Table 4. Characteristics of model diesel fuel

The number of the narrow fraction	Boiling limits of the narrow fraction, °C	Fraction content in raw materials, wt. %	The number of organosulfur components in the fraction	Pseudo component number	Conditional constant reaction rates of hydrodesulfurization, h^{-1}
1	180-240	50	14	1	15
2	240-320	25	14	2	9
3	320-350	10	3	3	5
4	350-365	15	2	4	1

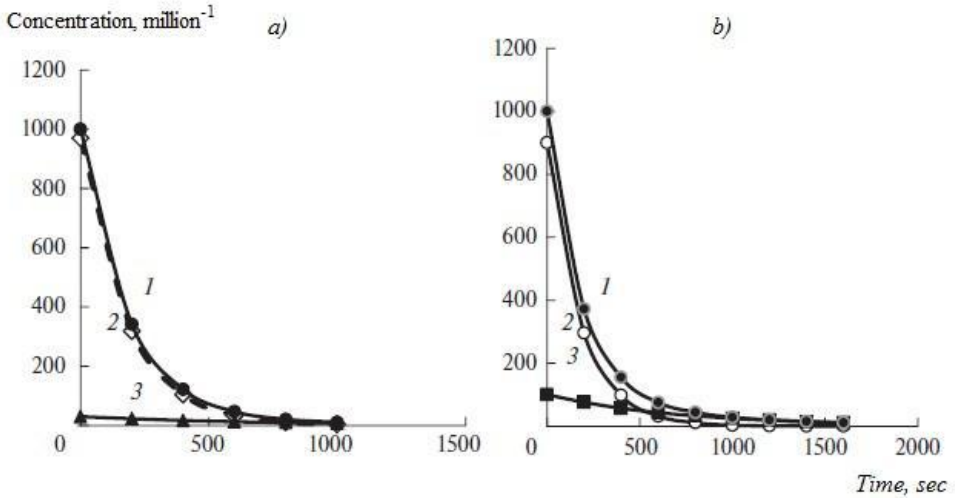

Fig. 4. Examples of calculating the kinetics of hydrotreating model diesel fuel with the proportion of a difficult-to-hydrogenate component in the total amount of sulfur-containing substances Z = 0.03 (a) and 0.1 (b): 1 – the total content of organosulfur substances; 2 – easily hydrogenated substances; 3 – difficult-to-hydrogenate substances.

The simulation results showed that as the concentration of hard-to-hydrogenate organosulfur substances in heavy fractions increases, the temperature boundary of the division of raw materials into light and heavy fractions shifts to a zone of lower temperatures. For example, with an increase in the concentration of the most difficult–to-hydrogenate pseudocomponent 4 from 500 (Table 5, series of experiments C) to 20,000 million^{-1} (Table 5, series of experiments B), the optimal boundary of the division of light and heavy fractions, which reduces the total volume of the catalyst in two reactors, shifts from the zone between components 2 and 3 (320°C) per zone between components 3 and 4 (350°C). The simulated systems for the concentration of organosulfur substances are quite typical for hydrotreated diesel fuels, for example, for straight-run diesel fuel from the diesel fuel hydrotreating plant G-43–107M/1 (fraction 180-365°C) with a total sulfur content of 24800 mln^{-1} when divided into fractions 180-320 °C (78 wt. %) and 320-365°C (22 wt. %) the total sulfur content in these fractions was 21700 and 32700 mln^{-1}, respectively.

It is characteristic that under optimal process conditions, the volumes of the catalyst loaded into each of the reactors are close to each other, which makes it possible to form a reaction unit of a hydrotreating plant from two identical reactors, compensating for some underloading or overloading of the catalyst compared to the required additional temperature control in each of the reactors.

Thus, the optimal position of the temperature boundary of the division of the feedstock into light and heavy fractions is determined simultaneously by the concentration and rate of reactions hydrodesulfurization of organosulphurization of organosulphurization components, while the temperature boundary of the division of raw materials can shift both upwards and downwards depending on the composition of organosulphurization impurities in the raw materials, while minimizing the criterion of optimality of the hydrotreating process, which can be taken as the minimum total loading of the catalyst into two reactors, characterizing the efficiency of the process [30].

When dividing the initial diesel fuel into two fractions, it is desirable to consider complexes of organosulfur substances in the form of at least four to six pseudo-components distributed in

corresponding narrow fractions, which together form two hydrotreated fractions. It should be noted that when characterizing raw materials by organosulfur components, six pseudo-components ensure acceptable accuracy of process modeling hydrotreating [31]. Naturally, an increase in the number of pseudo-components leads to an increase in the volume of experiments conducted to generate the initial data necessary for mathematical modeling of the hydrotreating process. At the same time, it is necessary to form model mixtures using expensive samples of specific organosulfur components. The optimization problem is much easier to solve if non-specific groups of homologues of organosulfur components are considered as pseudocomponents, as proposed in the hydrotreating of the entire raw material stream in [15, 22, 31], since organosulfur components that are fundamentally different in structure and reactivity may have similar boiling points (for example, 2-phenylthiophene and h-undecyl mercaptan have boiling points of 256 and 257°C, respectively), and consider the pseudocomponent as a set of organics to determine the parameters of the Arrhenius equation for the hydrodesulfurization reaction of this fraction of the initial diesel fuel in total sulfur from several experiments at different process temperatures.

3. Results and discussion

The loading of the catalyst with separate feeding into two reactors of light and heavy fractions is 2-3 times less than when feeding raw materials into one reactor or two sequentially or parallel reactors (Fig. 5), and as the concentration of organosulfur substances in the raw materials increases, this ratio increases.

Since the fractionation of the feedstock into light and heavy fractions requires additional energy consumption for heat supply and irrigation in the distillation column and subsequent heating of the resulting light fraction, compensating for the heat removal in the distillation column for the preparation of two fractions of raw materials, it is in principle possible to exclude this column from the scheme of the hydrotreating plant to obtain two fractions of diesel fuel with a given temperature the boundary of the fraction division directly at the primary oil refining plant [32]. In this case, the energy consumption for The hydrotreating unit will be even slightly lower compared to common schemes (Fig. 3a–3d) due to the receipt of two sufficiently hot fractions with a temperature of 150-200°C to the hydrotreating unit.

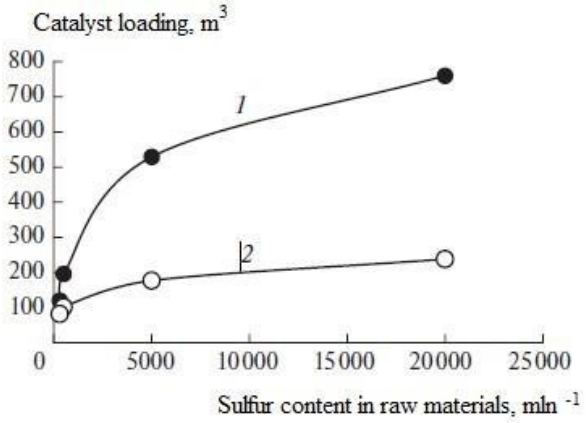

Fig. 5. The dependence of the catalyst loading into the reactor system of the hydrotreating plant on the sulfur concentration in the initial diesel fuel:
1 – a single reactor, two reactors operating in series or in parallel, 2 – the supply of light and heavy fractions of raw materials separately into two reactors.

Table 5. The results of modeling the operation of a two-reactor hydrotreating scheme for diesel fuel consisting of four pseudo-components

Option number	Pseudocomponents in the reaction mixture		The residence time of the product in the reactor, h		Catalyst loading, m^3			Sulfur concentration at the reactor outlet, mln^{-1}	
	Reactor 1	Reactor 2	Reactor 1	Reactor 2	Reactor 1	Reactor 2	Total	Reactor 1	Reactor 2
A	The concentration of pseudocomponents, $million^{-1}$: $C_1 = 12000$, $C_2 = 8000$, $C_3 = 3000$, $C_4 = 5000$								
1	1,2,3,4	-	5.29	-	529.50	-	529.50	9.99	-
2	**1,2,3**	**4**	**1.14**	**5.29**	**97.24**	**79.43**	**176.67**	**9.99**	**9.99**
3	1,2	3,4	0.74	5.29	55.65	132.40	188.05	9.78	9.99
4	1	2,3,4	0.47	5.29	23.50	264.50	288.00	9.87	9.99
B	The concentration of pseudocomponents, $million^{-1}$: $C_1 = 5000$, $C_2 = 10000$, $C_3 = 15000$, $C_4 = 20000$								
1	1,2,3,4	-	7.59	-	760.0	-	760.0	9.99	-
2	**1,2,3**	**4**	**1.46**	**7.59**	**124.1**	**113.9**	**238.0**	**9.95**	**9.99**
3	1,2	3,4	0.76	7.59	58.4	189.9	248.3	9.91	9.99
4	1	2,3,4	0.41	7.59	20.6	379.9	400.5	9.88	9.99
C	The concentration of pseudocomponents, $million^{-1}$: $C_1 = 20000$, $C_2 = 5000$, $C_3 = 2000$, $C_4 = 500$								
1	1,2,3,4	-	1.96	-	196.00	-	196.00	9.89	-
2	1,2,3	4	1.07	1.96	90.95	29.40	120.35	9.37	9.89
3	**1,2**	**3,4**	**0.70**	**1.6**	**52.50**	**49.00**	**101.50**	**8.93**	**9.89**
4	1	2,3,4	0.51	1.96	25.50	98.00	123.50	8.98	9.89
D	The concentration of pseudocomponents, million–1: $C_1 = 30{,}000$, $C_2 = 3000$, $C_3 = 300$, $C_4 = 100$								
1	1,2,3,4	-	1.20	-	120.0	-	120.0	9.84	-
2	1,2,3	4	0.80	1.20	68.0	18.0	96.0	7.01	9.83
3	**1,2**	**3,4**	**0.70**	**1.20**	**52.5**	**30.0**	**82.5**	**6.11**	**9.83**
4	1	2,3,4	0.60	1.20	30.0	60.0	90.0	4.05	9.83

4. Conclusion

For a comparative analysis of the efficiency of the reactor unit of diesel fuel hydrotreating plants by mathematical modeling, the loading of a catalyst into the reactor unit is considered as an optimality criterion, all other things being equal a process with the representation of a set of organosulfur components of raw materials in the form of several conditional pseudo-components. Of the considered options for the hardware design of the reactor unit in the form of a flow reactor, a reactor with recirculation of a part of the hydrotreated fuel, two reactors with sequential and parallel operation of reactors and two separately operating reactors with loading of light and heavy fractions of pre-separated raw diesel fuel, the lowest catalyst loading is provided in the last two-reactor version, while amounting to 70 to 30% compared to other options.

To substantiate the temperature boundary of the division of hydrotreating raw materials into light and heavy fractions, it is necessary to pre-divide the raw materials into 4-6 narrow fractions, in each of which the set of organosulfur components is considered as a pseudo-component, for which the kinetic characteristics necessary for the computational analysis of the hydrotreating process are experimentally determined.

Conflict of interest

The authors declare that they have no conflict of interest in relation to this research.

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