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Mathematical modeling of the process of catalytic hydrodewaxing of atmospheric gasoil considering the interconnection of the technological scheme devices

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Abstract

The authors proposed a mathematical model of the reactor of hydrodewaxing process and methodology to address the relationship of processes and devices for predicting the hydrodewaxing reactor operation and the related apparatus - stabilization column of the gas-product mix in order to use them to predict resource-efficient modes of the equipment operation. The influence of the downstream stabilization column composition of raw materials and quality of stable hydrogenate in order to determine the optimal irrigation flow into the column to increase the separation of hydrogen sulfide and light hydrocarbons by the top of the column is shown.

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Keywords: catalytic hydrodewaxing; mathematical model; HYSYS; otimization; raw material components

1. Introduction

The catalytic hydrodewaxing is aimed to produce low-sulfur summer, winter and arctic diesel fuel feedstock by hydrotreating followed by hydrocracking and hydroisomerisation of high-normal paraffins present in the diesel fraction, atmospheric gas oil and heavy visbreaking gasoline [1].

Mathematical models are used effectively in solving the problems of complex multi-component industrial processes of refining and petrochemistry optimization [2-5]. Within the catalytic hydrodewaxing process, models of

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hydrocracking / hydroisomerization of heavy products of the synthesis of Fisher-Tropsch process [6-8], of atmospheric residue [9], vacuum residue [10], vacuum gas oil [11], hydrocracking of n-decane taken as a model of raw material [12] have been developed so far. A significant number of works are devoted to the development of new catalysts [13-16], as well as to the study of the influence of the catalyst pore size and grain shape, the ratio of the acid and the metal as a catalyst in the reaction mechanisms of hydrocracking and hydroisomerization, yield and the composition of the finished product [17-21].

The industrial realization of the process is a sequence of related technological steps, each considerably determining the properties of the end desired products. At the same time, in order to save enterprise resources, the equipment of industrial plants should be operated efficiently, i.e. the modes of the devices should be optimized depending on the composition of raw materials with the contingency of the technological equipment [22].

After the reactor stage of hydrodewaxing, gas-product mixture is supplied into the stabilization column. However, the current mode of operation of the stabilization column is unsatisfactory. Firstly, light petrol of column C-1 and stable gasoline of column C-2 do not differ in composition. Secondly, there is a high content of hydrogen sulphide in the stable gasoline of column C-2, and in that case it cannot be recycled at the catalytic reforming plant to produce high-octane components of commercial gasoline due to catalyst poisoning action on sulfur-containing compounds.

The reason of the problems described is weak separation of light components and hydrogen sulfide, passing away as an overhead product of the column in the composition of hydrocarbon gas.

The authors suggested the solving of these production problems by the developing and implementing the reactor model of the hydrodewaxing and considering the interaction of processes and devices for prediction of the hydrodewaxing reactor operation and the related apparatus – stabilization column of the gas-product mixture with the purpose to exploit them for predicting resource-efficient modes of the equipment operation, which provide the required amount of specified quality end products.

2. Study subject

The object of the study is the joint work of the reactor unit and the unit of stabilizing the product of the reactor unit (the unstable hydrogenate) at the industrial catalytic hydrodewaxing plant. Conjugate work scheme and hydrodewaxing reactor stabilization product column model is shown in Fig. 1.

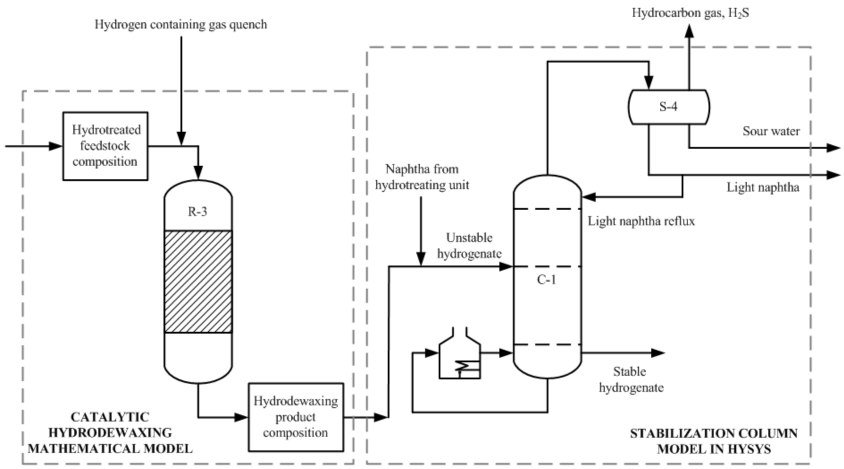

Fig. 1. Conjugate work scheme and hydrodewaxing reactor stabilization column model; C-1 – stabilization column; S-4 – separator

As it can be seen from Fig. 1, the composition of effluent flow is an input flow into the stabilization column. The study was conducted at the following process parameters: the unstable flow hydrogenation 312 m3 / h; consumption of gasoline, distillate 7.3 m3 / h; bottom temperature 323° C; top temperature of 100° C; bottom pressure 0.56 MPa; top pressure of 0.55 MPa.

3. Methods

In this paper, the following methods were used: quantum chemistry for calculating thermodynamic characteristics of reactions, occurring in the process of hydrodewaxing; mathematical modeling method, based on the system analysis strategy; modeling in HYSYS.

Mathematical modeling of catalytic hydrodewaxing is based on physical-and-chemical process characteristics: the mechanism of the reactions of cracking and isomerization on a bifunctional catalyst surface in hydrogen-containing gas medium is investigated and considered, calculations of thermodynamic reactions characteristics are conducted, process kinetic model is developed, and kinetic parameters are found. The model is checked for adequacy by comparing calculated values by composition product mixture and values, obtained in the process of correct industrial plant operation within a wide changing range composition feedstock and technological conditions [23].

4. Results and discussion

The study of the influence of the stabilization column composition feedstock on hydrogen sulfide and light paraffins yield as a part of hydrocarbon gas is carried out. Feedstock C-1 is a mixture of the reactor unit product, which composition is calculated by the hydrodewaxing process reactor mathematical model in relation to the feedstock composition, supplied to the plant, and process technological parameters, and naphtha. The feedstock compositions are given in table 1.

Table 1. Composition of the stabilization column feedstock

Indicator	Feedstock 1	Feedstock 2	Feedstock 3
ibp	106	97	108
30%	266	269	271
50%	292	294	296
70%	319	320	320
90%	352	350	350
fbp	377	371	371
H_2S, % wt.	0.0008	0.0041	0.0016

where ibp is initial boiling point, °C; fbp is final boiling point, °C.

Fig. 2 shows the yields by hydrogen sulfide and light paraffins feedstock within hydrocarbon gas and stable hydrogenate for the three feedstock compositions.

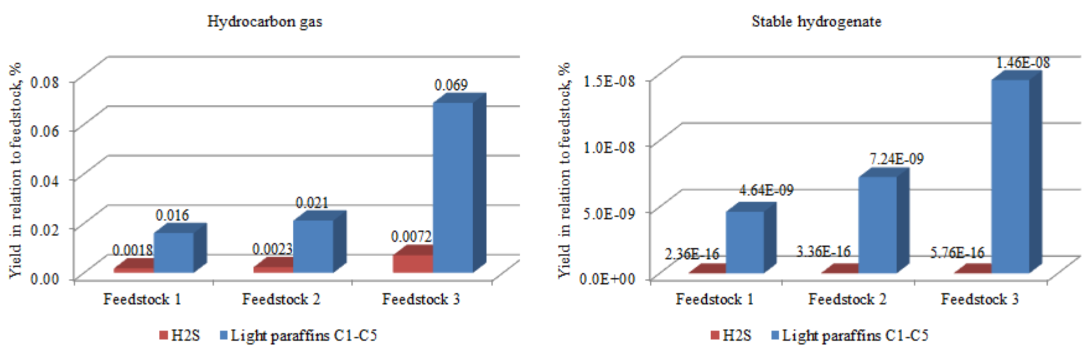

Fig. 2. The yield of hydrogen sulfide and light paraffins as a part of hydrocarbon gas and stable hydrogenate from column C-1 depending on the feedstock composition

As it can be seen from Fig. 2, feedstock composition considerably influences the hydrogen sulfide and light paraffins separation by the column top. For feedstock 3, maximum hydrogen sulfide and light paraffins yield with hydrocarbon gas is observed. At the same time, for this feedstock composition, maximum hydrogen sulfide and light paraffins C1-C5 yield within stable hydrogenate is observed. For keeping the required content of these components in stable hydrogenate it is necessary to provide optimal operating conditions for the stabilization column depending on the feedstock composition. In this study, quantity of reflux was chosen as a regulatory parameter.

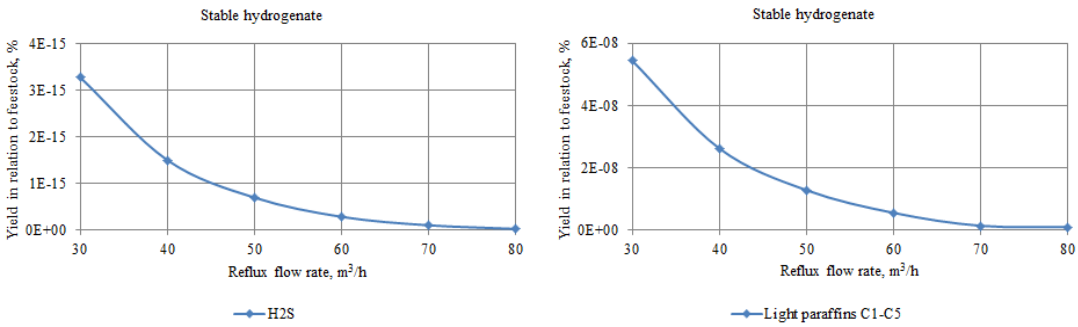

Fig. 3. The yield of hydrogen sulfide and light paraffins as a part of stable hydrogenate composition from column C-1, depending on the feed composition

Thus, for achieving planned yields of hydrogen sulphide and light paraffin for feedstock 3 it is necessary to keep the reflux rate at level 70 m^3/h (Fig. 3).

5. Conclusion

The conducted study has shown that for providing high yields of hydrogen sulphide and light paraffin by the top of the column as a part of the hydrocarbon gas, it is necessary to select the optimum operating parameters of the column C-1, taking into account the composition of the feedstock. This will more clearly separate the light fraction and stable gasoline, as well as receive stable gasoline with a minimum content of hydrogen sulphide (less than 0.00001% wt.) for its further processing at the reforming unit to produce high-octane components of gasoline.

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