SIMULATION OF ALKYLATION PRODUCTS PROCESSING TO STUDY THE DURATION OF PERIOD BETWEEN REACTOR WASHINGS

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Synthetic detergents are produced of linear alkylbenzenesulfonates (LABS). LABS are organic chemical compounds with long saturated hydrocarbon chain and one or several sulfonic acid groups. LABS are the key components of synthetic detergents and are obtained by following steps:

- dehydrogenation of alkanes on Pt-catalyst with olefins obtaining
- alkylation of benzene with obtaining of linear alkylbenzenes (LAB). The process runs using HF as catalyst;
- sulfonation of LAB with obtaining of ASA

Since the consumption of synthetic detergents produced on the basis of surfactants increases annually, the requirements for the production technology of components are increasing in terms of quality and economic benefits [1].

In order to avoid reducing the quality of the product and increasing the economic efficiency of the process, it is necessary to monitor the formation of a viscous component. During its accumulation, the uniformity of the organic film flow is disturbed and the diffusion of SO3 molecules slows down. As a result the process does not fully proceed, and the quality the products deteriorate. The purpose of this work is to simulate the processing of linear alkylbenzenes in a multi-tubular film reactor and use the computer simulation system to predict the duration of period between reactor washings based on the accumulation of a high-viscosity component [2–3].

The sulfonation runs in a multi-tubular film reactor. The process goes in a plug flow.

Kinetic coefficient of chemical reactions was found when solving the inverse kinetic problem (Table 1).

Table 1

Kinetic coefficient of base chemical reactions

№	Reaction	k
1	LAB + SO3 → ASA	6,25
2	LAB + ASA → non-sulf+ H2O	0,09
3	ASA + SO3 → ASA anhydride + H2SO4	3,87 · 10-4
4	non-sulf → highly viscous component	8,34 · 10-5

The calculations were performed using a computer simulation system based on data from real sulfonation process. As a result the dynamic of concentrations of key products such as ASA, non-sulfated component, H_2SO_4 was obtained.

The calculated data correlate with experimental ones, which means that the model is adequate and can be used to study the main parameters of the process. The results are performed in Figure 1.

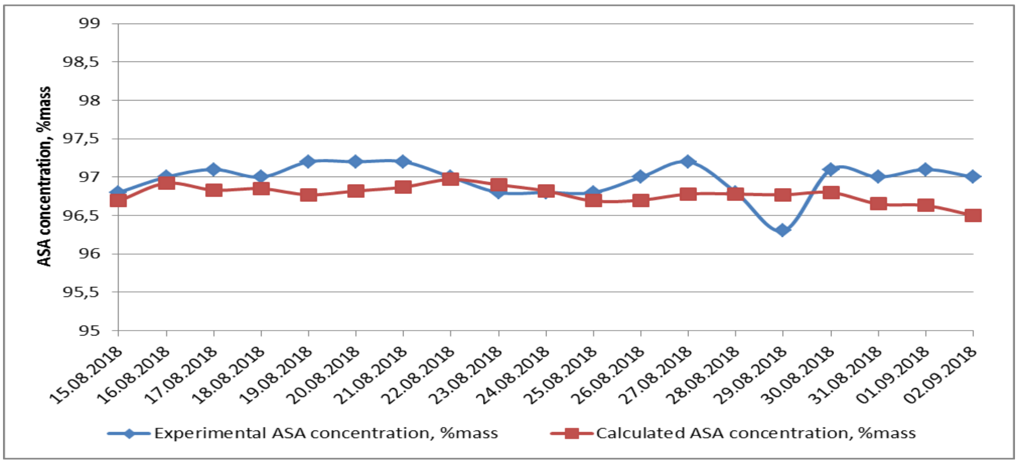

Fig 1. Dynamic of experimental and calculated concentrations of ASA

Now the necessity of reactor washing is determined by pressure value inside the reactor, which depends on concentration of highly viscous component accumulated. In practice, this method does not allow to achieve maximum efficiency of the process and is associated with the risk of the formation of an off-test product.

The use of a computer simulation system allows you to make predictions about the duration of the period between reactor washings based on the concentration of a highly viscous component.

The results of the calculation of a highly viscous component accumulation during one the period between reactor washings are presented in Figure 2.

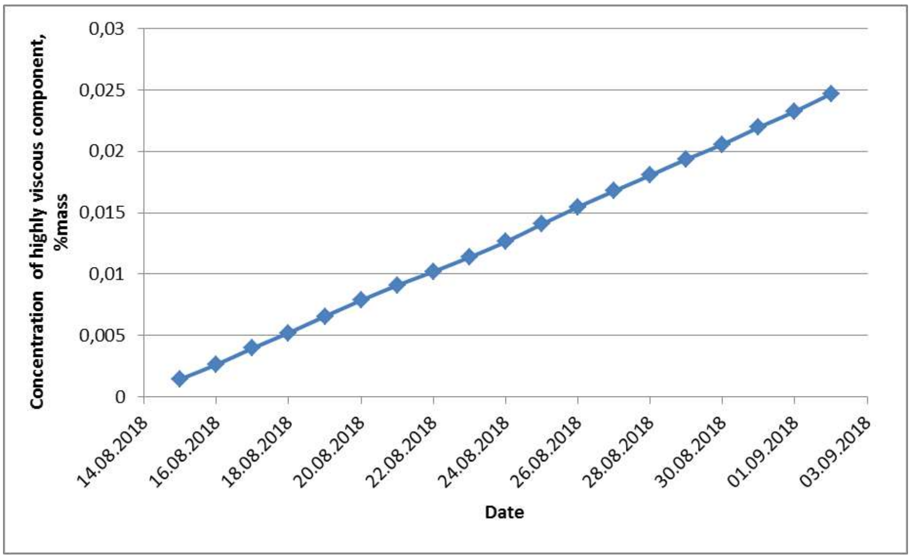

Fig 2. Dynamic of highly viscous component accumulation during one period between reactor washings

Thus, we can draw the conclusions that the developed model is adequate and able to calculate of the duration of period between reactor washings in the sulfonation reactor based on the accumulation of a high-viscosity component.

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References

1. Bannov, P.G. Processy pererabotki nefti. / P.G. Bannov. – M.: CNIITEHneftekhim. - 2001. – 625 p. [in Russian]
2. Dolganova I. O., Dolganov I. M., Bunaev A.A., Pasyukova M.A. Nature of highly viscous component in the alkylbenze sulfonic acid technology and its influence on the process efficiency [Electronic resorces] // Petroleum and Coal. – 2019 – Vol. 61 – №. 1. – pp. 25-31.
3. Dolganova I.O., Dolganov I.M., Ivanchina E.D., Ivashkina E.N. Alkylaromatics in Detergents Manufacture: Modeling and Optimizing Linear Alkylbenzene Sulfonation // Journal of Surfactants and Detergents. – 2018 – Vol. 21 – №. 1. – pp. 175-184.

DEVELOPMENT OF HEAVY OIL AND BITUMEN FIELDS WITH DIFFICULT CONSTRUCTION WELLS

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High-viscosity oils and natural bitumen should be considered as a complex raw material. They include valuable organic compounds, including naphthenic acids, metal porphyrins, ethers and esters, which can serve as a source of unique catalysts, etc. They find application in medicine, in chemical technologies, in biotechnologies, therefore the question of development of deposits of heavy oils is especially actual.

Over two trillion barrels of viscous oil (heavy oil, extra heavy oil, and bitumen) are contained in naturally fractured carbonate rocks [4]. Mobile bitumen lies in sand and siltstone reservoirs, more viscous in carbonate. The basis for the cost-effective development of bitumen production can be the joint operation of natural bitumen deposits and ultra-viscous oil deposits located at a depth of 800-1200 meters.

Known methods of extraction of heavy oils and bitumen are characterized by high energy costs of thermal influence. The main complicating factors are the low permeability of bitumen-containing reservoirs and the viscosity of products exceeding 1000 mPa*sec. The capabilities of standard equipment for mechanized production do not meet the requirements of the high-viscosity oil deposits development due to the action of hydrodynamic friction forces during the movement of liquid in pipes. Therefore, there is an improvement of existing technologies and complication of well design.

It is known a method of the heavy oil and bitumen fields development by double-well horizontal wells is, which increases the efficiency of their development [3]. The method is: the opening of the productive formation is carried out by a horizontal trunk and its fastening by a casing flow string, previously equipped with a filter in the interval of the opened productive formation, the equipment of the wellhead, the installation of a blind packer through one wellhead in the interval of the productive formation of the well corresponding to the contour of watering, and the operation of the well through the second wellhead with the use of a pump.

Therefore, one of the wellheads of the well is used for thermal and chemical exposure or geophysical research and the second one – for production of hydrocarbons (fig.1). The complexity of monitoring the parameters of the steam chamber