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THE STRUCTURAL DETERMINATION OF FLOWS IN THE SINGLESTAGE REACTOR FOR THE SULPHURIC ACID ALKYLATION[1](#page-0-0)

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Keywords: alkylation, reactor, flow structure, reactor geometry, cross-section, flow resistance Abstract. The article considers the flow sulphuric acid alkylation reactor designed to produce the high-octane component of petrol fractions and aviation fuel. The industrial application uses the narrow fractions containing the necessary hydrocarbons as raw materials. Isobutane has the greatest practical importance for alkylation but it is used as a raw material in relatively small quantities. The quality of the resulting alkylate decreases depending on the olefin used. The industrial plants implement new engineering measures to improve the technical and economic efficiency of the operations. Consequently, the main trends in the modern sulphuric acid alkylation process are: the construction of new high-capacity units based on advanced technologies; increase of raw material resources for alkylbenzene production; search for thecatalysts and new methods for alkylation of isobutane with olefins; development of highly efficient technologies.

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Introduction

Because of the higher quantities of isobutane and sulphuric acid used, the alkylation of isobutane with a butylene mixture, which can be produced in many large-scale secondary refinery processes, is preferred for the reactions in industry. The yield and quality of alkylation products is determined not only by the properties of the raw material and catalyst, but also by process parameters such as pressure, temperature, concentration of sulphuric acid, concentration of isobutane in the reaction zone, reaction time, etc. [1-3].

Reactor design has a particular influence on the process efficiency. Usually sulphuric acid alkylation is performed using vessel reactors with flow and mechanical stirring, with different ways of removing the excess heat from the reaction. The variety of reaction equipment designs is the result of a compromise between the cost of isobutane, acid, reaction time, and the quality of the alkylate produced.

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The main stages of the sulphuric acid alkylation process are shown in Figure 1. Modern plants usually use butane-butylene fraction as a raw material for alkylation. The technological scheme of sulphuric acid alkylation of butylenes consists of the following main stages: raw material preparation, reaction zone, processing of hydrocarbon mixture, product fractionation [4, 5].

There are currently many process schemes for the sulphuric acid alkylation process, but their operating principles are is similar. The raw mixture, recycled isobutane, and acid are pumped through pipes by circulating pumps and sprayed through nozzles into the reactor, producing the fine emulsion of the raw material and acid. Some of the mixture is led from the bottom of the reactor to a cooler to remove the heat of the alkylation with the coolant and is pumped back into the reactor pipes. The duration of a total circulation cycle is 1 to 2 minutes.

Fig. 1. The main stages of sulphuric acid alkylation

A part of the emulsion from the reactor is continuously discharged into a settling tank, where it is separated into hydrocarbons and acid. The hydrocarbons are the nonreacted part of the emulsion, and the alkylate, which are routed for fractionation. Acid returned to the reactor. The isobutane separated in the fractionation unit is also returned to the reactor [6].

The structural determination of flows in the reactor of the sulphuric acid alkylation

The operating experience of the operating flow alkylation reactor since 2010 at unit 25/7 of JSC "Slavneft-YaNOS" demonstrated a rather low value of the ejection coefficient (1.5-1.8) [1-4]. The cause was the increased hydraulic resistance to circulation flow in some parts of the reactor, particularly in the nozzle areas [1, 7, 10, 11]. There is also the influence of the flow breakaway zones at the inlet to the inner circulation pipe, as well as the viscous wall friction caused by the high content of concentrated sulphuric acid [1-10].

To reduce the hydraulic resistance to the circulation flow within the modification of the tray + nozzles element only, we proposed to use smaller nozzles by reducing their height (300 mm instead of 340 mm) while keeping the diameters of the shear nozzle (55 mm) and inlet [1].

For this purpose, we carried out a modelling of the reactor interior hydrodynamic environment. We designed a 3D model of the flow reactor using modern CAD systems, created a design grid with the required element parameters, and carried out a numerical calculation. Figure 2 shows a scheme of the reactor and a fragment of an irregular T-sieve on its surface.

Fig. 2. Reactor geometry and calculation grid: *a* - cut control sections; *b* - sectional geometry; *c* - irregular T-mesh on product surface

Some calculation results:

ejection coefficient $K = 2.2 - 2.5$ (variation depends on the choice of turbulence model, for the model k- ε - 2.5) (minimum increase of at least 30%);

speed at the nozzle tip 14 m/s;

pressure differential at the nozzle 1.5 atm (previous version 0.6 atm);

residence time - maximum 42 s, average 12 s;

We obtain the numerical results presented for this reactor using the OpenCFDLimited software. The current lines and velocity isocontours in the reactor control sections are shown in Fig. 3-6.

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Fig. 3. Flow lines in the cross sections **Fig. 4.** Detailed flow structures

Fig. 5. Reagent mixing zones in the reactor **Fig. 6.** Detailing of flow lines in longitudinal and cross-sections of the reactor

Conclusion

We can conclude that:

The presence of longitudinal eddies leading to rip currents at the inlet of the circulation pipe from below and the outlet from above;

The formation of transverse vortices around the nozzles of the emulsification lattice and in the conical transition at the outlet of the dispersion zone leads to different residence times of the components in the reaction volume and the formation of by-products;

The high resistance of the nozzle grate leads to a reduction in capacity, increasing the areas of low mixing intensity;

Low efficiency of the olefin feeder collector distribution units; Imperfect design of the lower grille nozzles.

References

- 1. **Dolgin, D.S., Gudanov, I.S., Lebedev, A.E., & Vatagin, A.A.** (2022) On the case study of increasing the efficiency of a flow reactor for sulphuric acid alkylation, *Chimicheskoe i neftegazovow mashinostroenie*, 7, pp. 7-9 (in Russian)
- 2. **Gudanov, I.S., Lebedev, A.E., Kapranova, A.B., Sibrina, T.M. & Vinogradova, E.A.** (2021) Mathematical model of a flow structure in pulsation crystallizer, *From Сhemistry Towards Technology Step-by-Step,* 2(1), pp. 91-102 [online]. Available at: http: //chemintech.r[u/index.php/tor/2021tom2no1](http://chemintech.ru/index.php/tor/2021tom2no1) (accessed 12.11.2022). DOI: 10.52957/27821900_2021_01_86.
- 3. **Gudanov, I.S., Lebedev, A.S., Vatagin, A.A. & Dolgin, D.S.** (2018) Development of highly efficient design of a flow reactor for sulfuric acid alkylation, *Ingenerniy Vestnik Dona,* 4 [online]. Available at: http://www.ivdon.ru/ru/magazine/archive/n4y2018/5262 (accessed 12.11.2022) (in Russian).
- 4. **Gudanov, I.S., Lebedev, A.E. & Dolgin, D.S.** (2020) Problem of Updating Design of Horizontal Cascade Reactor for Sulfuric Acid Alkylation of Isoparaffins by Olefins, *Chemical and Petroleum Engineering*, 55(11-12), pp. 958-962. [online]. Available at: <https://link.springer.com/article/10.1007/s10556-020-00720-z> DOI 10.1007/s10556-020-00720-z
- 5. JSC "Slavneft-Yaroslavnefteorgsintez". (2003) *Technological regulations for the sulphuric acid alkylation plant.* Yaroslavl (in Russian).
- 6. **Kozlov, B.I.** (1990) *Alkylation, isomerisation and polymerisation processes in oil refining*. M.: Khimiya (in Russian).
- 7. **Kapranova, A.B., Lebedev, A.E., Melzer, A.M., Neklyudov, S.V., & Brykalov, A.S.** (2021) Analysis of basic characteristics of fluid throttling in a regulating axial valve, *From Chemistry Towards Technology Step-by-Step*, 1, pp. 104-112 [online]. Available at: http: /[/chemintech.ru/index.php/tor/2021tom2no1](http://chemintech.ru/index.php/tor/2021tom2no1) (accessed 12.11.2022). DOI: 10.52957/27821900_2021_01_86 (in Russian).
- 8. **Timonin, A.S.** (2002) *Fundamentals of design and calculation of chemical engineering and environmental protection equipment: Reference book. 2nd edition, revised and extended*. Kaluga (in Russian).
- 9. **Akhmetov, S.A.** (2002) *Technology of deep oil and gas refining*. Ufa: Gilem (in Russian).
- 10. **Kozin, V.G., Solodova, N.L., Bashkirtseva, N.Yu. & Abdullin, A.I.** (2008) *Modern Technologies of Motor Fuels Components Production*. Kazan: KSTU (in Russian).
- 11. **Romanov, I.A.** (2006) *Gasoline Production*. M.: Stroyizdat (in Russian).

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