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Modeling of Transalkylation Stage of Ethylbenzene Manufacturing with Zeolite-Catalysts

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Abstract

The analysis of industrial transalkylation reactor revealed regularities of catalyst activity and stability changes during its operation at change of basic technological parameters. A result of experimental data analysis, a list of possible reactions of transalkylation stage of ethylbenzene manufacturing zeolite-catalyst technology was developed. Values of Gibbs energies for change targets and adverse reactions, which were calculated with use of quantum chemistry methods, confirmed their thermodynamic probability at process conditions. The calculation results formed the basis of transalkylation process reaction network, needed to develop a mathematical model of ethylbenzene manufacturing zeolite-catalyst industrial technology.

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Keywords: Transalkylation; mathematical model; zeolite-catalyst

1. Introduction

The process of production of ethylbenzene (EB) is an important link in modern petrochemical synthesis. More than 90% of EB produced is recycled to styrene, one of the most important chemical products, about 65% of which is used for production of polystyrene, which is widely used in automotive industry, electrical engineering and construction industry, electrical engineering, in the manufacture of household products and packaging, as well as during the coproduction of propylene oxide and styrene [1].

Currently, there is a trend for existing plants to use modern solid alkylation zeolite catalysts. That is why the problem of existing plants efficiency enhancing is urgent [1-5].

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Zeolite catalysts for the process of benzene alkylation and di- and polyalkylbenzenes (PEB) transalkylation were first developed in mid 60-ies of the last century.

To date, several large companies such as Mobil, UOP / Lummus, Polimeri Europa, CDTECH and others, develop and implement ethylbenzene manufacturing processes.

In order to optimize and increase the process efficiency, mathematical modeling method is widely used. It not only saves time and money for testing, but also has a high parameter sensitivity [6-13]. A mathematical model of industrial reactor process, to be predictive, should consider physical and chemical laws. When modeling it is necessary to use data from existing industrial installations, which will provide a high value for the model.

The aim of this work was to develop transalkylation process reaction network needed to develop a mathematical model of ethylbenzene manufacturing zeolite-catalyst technology, on the basis of industrial reactor analysis and in combination with quantum-chemical modeling method of.

2. Study object

The object of research is transalkylation reactor of ethylbenzene manufacturing plant by EBMax technology [14].

3. Methods

Studies are based on system analysis strategy. The chemical-technological system for ethylbenzene production was decomposed into hierarchical stages. We determined the links between the levels: molecular level (the mechanism of catalytic reactions), physical and chemical processes in the devices, the links of processes and devices in the whole chemical-technological system. The main methods of system analysis strategies are mathematical modeling and quantum chemistry methods for calculation of thermodynamic characteristics of transition states of matter (density functional theory). For numerical investigation of catalytic process we used DFT method based on density functional theory (DFT-Density Functional Theory), which consideres the effect of electron correlation [15-17]. The method is implemented in Gaussian-98 application.

We used statistical methods to assess the model calculations accuracy and analysis of transalkylation reactor monitoring data during its operating period since 2013 to 2015.

4. Experimental

Polyethylbenzenes (PEB) are mainly diethylbenzene (DEB), and triethylbenzene, witch can be transformed into through transalkylation. This transalkylation reaction occurs in the liquid phase. Transalkylation reactor comprises a fixed bed EBMax transalkylation catalyst layer supported on alumina balls. Reactants enter the bottom of the reactor (Fig. 1). The process conditions are about 200 °C and 3.4 MPa.

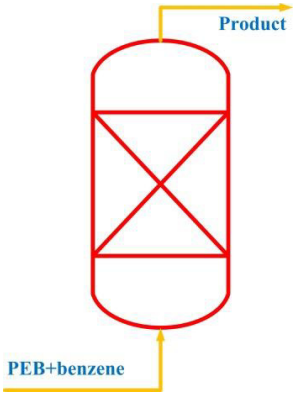

Fig. 1. Transalkylation reactor scheme.