



Alkylation of benzene with ethylene in the presence of dimethyldichlorosilane



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ABSTRACT

The kinetics of the alkylation of benzene with ethylene in the presence of dimethyldichlorosilane (DMDCS) are studied and a kinetic equation for this homogeneous irreversible reaction of the second order is created. The circulation of the DMDCS catalyst does not reduce its initial activity in relation to the formation of ethylbenzene and diethylbenzenes. The presence of moisture in the initial $C_6H_6 + C_2H_4 + DMDCS$ mixture reduces the catalyst activity. The dehydration of the starting mixture by removal of moisture from benzene was carried out using an azeotropic distillation. A reaction mechanism for the benzene alkylation with ethylene in the presence of DMDCS is formulated based on the generalized quantum-chemical principle and the theory of groups. The participation of DMDCS in the process of hydrocarbon conversion is confirmed experimentally and theoretically for the first time.

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1. Introduction

Ethylbenzene (ETB) is a product that is manufactured in excess of several million tons per year. It is used for the production of styrene, its polymers and copolymers, as well as chlorine- and oxygen-containing compounds, and other products [1]. Scientists worldwide have carried out research aimed at the improvement of the production process of ETB through the development of new catalysts and technologies for the alkylation of benzene with ethylene.

The industrial alkylation process of benzene with ethylene, outlined in 1877 by the studies of Friedel, Crafts, and Gustavson, is conducted on polyalkylbenzene in the presence of an aluminum chloride complex.

Approximately 50% of ethylbenzene is produced in the presence of the $Al_2Cl_6 \cdot nArR$ complex. This technology has been implemented and described in articles and monographs by several research groups [1–5].

An important direction of the work of both research groups and educational institutions is the development of effective aluminosilicate zeolites as catalysts for benzene alkylation [6,7].

The number of scientific publications reflects the great deal of research work that has been performed on the alkylation of benzene with ethylene in the presence of homogeneous and heterogeneous catalytic systems [8–22].

The investigation of the alkylation of benzene with ethylene over the faujasite zeolite by the ONIOM method has been described [8]. Beta, MCM-22, USY-1, and USY-2 zeolites have been shown to efficiently activate the C_6H_6 and C_2H_4 molecules for the alkylation of benzene with ethylene in the liquid phase, under pressure and at low temperatures [9]. It has been established that the zeolite activity increases in the order $MCM-22 > Beta > USY-1 > USY-2$ [18].

In another study, the usage of tablets of clay mixed with aluminum oxide as active catalyst has been described [10].

It has also been established that the reasonable processing of the zeolites MCM-49 and MCM-22 in a 0.025 N sodium hydroxide solution increases the selectivity of the catalyst to ETB up to 97% at $P = 3.5$ MPa and $T = 493$ K in the liquid phase [11].

In another reports, the authors postulated that the weak and strong catalytic centers of the MCM-56 zeolite might participate in the catalytic alkylation process [12,13].

The zeolite β exhibits an enhanced catalytic activity [14]. The zeolite MCM-49 possesses a high selectivity, and a correlation has been found between the activity and the content of the Brønsted centers on the zeolite surface and in its lattice [15].

The oxidative alkylation of benzene with ethylene is effective over the ZSM-5 zeolite. [16]. The ETB selectivity in the liquid phase

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