

# Joint synthesis of methyl ethyl ketone and phenol based on oxidative transformations of *sec*-butylbenzene

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**The relevance of the work.** Methyl ethyl ketone (MEK) is a commercially important product of basic organic and petrochemical synthesis. This compound is widely used as an extractant in the processes of dewaxing lubricating oil and degreasing agent for metal surfaces and electronic devices. Having a good solvent ability in relation to many substances, MEK is used in the production of paint, polymer and building materials and coatings, adhesives. In the pharmaceutical industry, MEK is used in conjunction with alcohols in the production of antiseptics and some medicines.

In laboratory chemical analysis, it is known to be used in quality control of finished products according to the indicator "Residual organic solvents" by gas chromatography. MEK is also an intermediate product in the synthesis of other organic compounds.

Currently, there are two industrial methods for the production of MEK, consisting in the production of butanol-2 by sulfuric acid or direct hydration of *n*-butylene followed by catalytic oxidation in the presence of silver on a zeolite carrier or alcohol dehydrogenation using zinc-copper catalysts. The main disadvantages of these processes are their implementation in harsh conditions (at a temperature of 480-550 ° C), the use of expensive catalytic systems, low productivity and high energy consumption. In addition, it is worth noting that the technologies for obtaining MEK are implemented only in Western Europe, Latin America and Asia. The needs of Russian enterprises are almost completely met by foreign supplies, which is why the MEK, according to data for 2024, is included in the List of critical components.

The above circumstances determine the urgency of conducting research aimed at developing an alternative technology to the existing production of MEK based on available petrochemical raw materials based on the liquid-phase oxidation of *sec*-butylbenzene to its hydroperoxide, which is subjected to acid decomposition into target products. The developed method allows, along with MEK, to obtain phenol, which is widely used in the production of plastics and synthetic fibers, pesticides, various explosives, dyes and textiles, as well as quite often used in the manufacture of medicines.

**The purpose and tasks of the work.** To develop the scientific and applied fundamentals of chemistry and technology of the hydroperoxide method for the joint production of MEK and phenol based on available petrochemical raw materials.

To achieve this goal of the work, the following tasks are set:

- to study the regularities of the synthesis of *sec*-butylbenzene by the alkylation reaction;
- to investigate the regularities of the process of aerobic liquid-phase oxidation of *sec*-butylbenzene to hydroperoxide;
- to make a kinetic model of the process of liquid-phase oxidation of *sec*-butylbenzene to hydroperoxide in the presence of *N*-hydroxyphthalimide;
- to study the influence of the main parameters on the process of acid decomposition of *sec*-butylbenzene hydroperoxide to MEK and phenol;

- to make a kinetic model of acid decomposition of *sec*-butylbenzene hydroperoxide.

**Scientific novelty.** A method for obtaining MEK together with phenol based on the hydroperoxide oxidation of *sec*-butylbenzene in the presence of *N*-hydroxyphthalimide has been proposed and experimentally substantiated. For the first time, regularities of the main stages of the process under development have been obtained and the best conditions for their implementation have been determined.

The regularities of the reaction of aerobic liquid-phase oxidation of *sec*-butylbenzene to its *tert*-hydroperoxide have been investigated. For the first time, an experimental assessment of the relative reactivity of *sec*-butylbenzene in a liquid-phase oxidation reaction was carried out by determining the parameter  $(k_2/\sqrt{2k_6})$ . It has been shown that *sec*-butylbenzene has a lower reactivity compared to its closest homologue isopropylbenzene. It has been established that the use of organic *N*-hydroxyphthalimide catalysts makes it possible to significantly intensify the process under study in comparison with the initiated oxidation of *sec*-butylbenzene. The kinetic patterns of *sec*-butylbenzene oxidation in the presence of *N*-hydroxyphthalimide have been studied and a mathematical model has been compiled that adequately describes this process. The influence of temperature, catalyst concentration, and initial concentration of *sec*-butylbenzene hydroperoxide on the process of its acid decomposition into target products has been studied.

**Practical significance of the work.** The results of the conducted research confirm the technological effectiveness of the developed method of obtaining MEK in comparison with alternative methods of synthesis of this product. The mechanism of catalytic oxidation of *sec*-butylbenzene to hydroperoxide in the presence of *N*-hydroxyphthalimide is discussed. It was found that the use of this catalyst in the oxidation process makes it possible to achieve a 35-40 % conversion of *sec*-butylbenzene with a selectivity of *sec*-butylbenzene hydroperoxide formation above 95 %. Based on the proposed reaction mechanism, a kinetic model has been compiled that can be used to make the hardware design of this process. The conditions allowing to synthesize high purity MEK and phenol with yields of 72 and 74 %, respectively, were found. The proposed hydroperoxide method for the joint production of these products makes it possible to expand the potential of this method by adapting cumulus technology to produce a wide range of phenols and ketones, depending on the specifics of the chemical products market in certain regions of the Russian Federation.

**Provisions to be defended:**

1. A method for the joint production of MEK and phenol based on the hydroperoxide oxidation of *sec*-butylbenzene, including the synthesis of *sec*-butylbenzene, its aerobic liquid-phase oxidation to hydroperoxide and the acid decomposition of the latter into target products.
2. Regularities of the reaction of aerobic liquid-phase oxidation of *sec*-butylbenzene to hydroperoxide.
3. Substantiation of the role of *N*-hydroxyphthalimide and its derivatives in the oxidation process *sec*-butylbenzene to hydroperoxide.
4. Regularities of acid catalytic decomposition of *sec*-butylbenzene hydroperoxide in MEK and phenol.