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ABSTRACTS

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- **Section I.** Advances in Chemical Reactors Fundamentals;
- **Section II.** Chemical Reaction Engineering and Reactors Design – Novel Approaches, Modeling, Scale-Up, Optimization;
- **Section III.** Chemical Reactors and Technologies for Emerging Applications;
- **Section IV.** Advanced Processing of Fossil Hydrocarbon Feedstocks;
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NUMERICAL SIMULATION OF THE FLUIDIZED BED CHEMICAL REACTOR WITH STRUCTURAL ELEMENTS OPTIMIZATION

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Isobutylene is an important monomer for petrochemical synthesis. On the basis of isobutylene a wide range of materials is obtained, such as synthetic rubbers, films and fibers, high-octane components of gasoline. The main method of isobutylene producing in Russian Federation is the isobutane dehydrogenation in a fluidized bed of catalyst. The catalyst is a complex system consisting of an alumina support and deposited on its surface the active component – Cr_2O_3 and the promoter – K_2O. High activity of alumina-chromia catalyst is detected in the dehydrogenation of isobutane in the laboratory conditions, but not always in the conditions of industrial application. This may be caused by the temperature of the catalyst bed, which is not sufficient to provide a high conversion of isobutane in the endothermic dehydrogenation reaction. To maintain the required temperature, it is necessary to feed of heated catalyst in a fluidized bed. The main task is the effective heating of zone of the fluidized bed with the highest concentration of catalyst.

Currently, one of the ways to determine the properties of large-scale fluidized beds is numerical simulation. In a study of fluidization was extended Eulerian-Eulerian approach, when carrier phase (gas, liquid) and discrete (solid) phase is continuous. To account for movement of features in a fluidized bed, using the kinetic theory of gases added to the equation describing the change in kinetic energy of the granules in consequence of collisions.

This paper presents the results of calculations of chemical reactor with a fluidized bed of pulverized catalyst. The hydrodynamics and heat transfer in a chemical reactor model based on existing industrial unit dehydrogenation of isobutane was studied. In the lower part of the reactor feeder gas feedstock is situated. In the center of reactor there is a vertical pipe feeding from the regenerator. A regenerated heated fresh catalyst is feeding to the zone above the upper grid. Calculations were performed using numerical methods of computing.

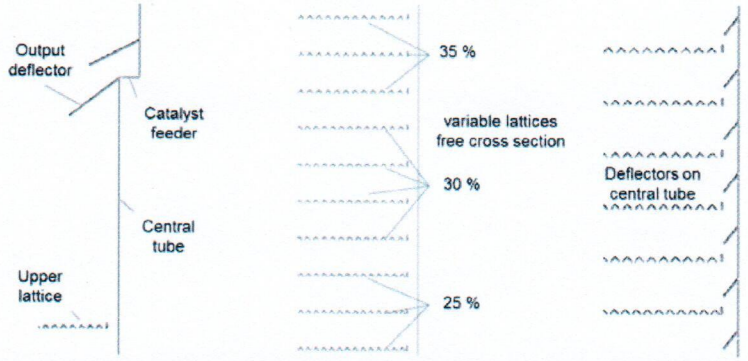

Figure 1. Variants of structural elements modification

Each structural element of the specific apparatus may become critical to overall efficiency. To increase heat transfer in areas of high catalyst concentration were made calculations of reactor with different design variants. There are an "output deflector" in the output of the catalyst feeder; variations of the free cross section of lattices in the reactor; deflectors on the central tube in the lattices zone (Figure 1).

Fields of catalyst concentration, temperature and the function of the chemical reaction efficiency field (which depends on temperature and catalyst concentration) were obtained (Figure 2). The directions and options for modifications are determined that increase the efficiency of the investigated chemical reactor.

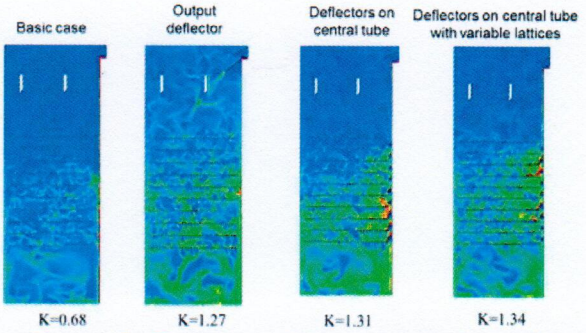

Figure 2. Function of the chemical reaction efficiency fields, K – efficiency coefficient

Various modifications in the wide range of the fractional composition of the catalyst show different efficiency. Since an increase in small particles some modifications provide to increase the probability of chemical reaction, and others – decreasing. Most effective for the investigated reactor is deflecting elements for the central tube with a simultaneous increase of the lattices free cross section in elevation.