Title of the PhD thesis:

Analysis, modelling and simulation of ethanol conversion to 1,3-butadiene process

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Abstract

The objective of the research carried out during the doctoral studies was the analysis of the of ethanol conversion into 1,3-Butadiene (BD) process (ETB process), by the single-step technology (Lebedev), to develop procedures useful in the design of fixed-bed catalytic reactors, for this process. From a chemical point of view, the ETB transformation consists of a complex consecutive-parallel reactions system. The main results reported in the thesis refer to: (i) an extensive review of published studies regarding the catalysts proposed for this transformation, the process thermodynamics and process kinetics; (ii) an ETB process thermodynamic study, including the spontaneity of the transformation and the chemical equilibrium state particularities; (iii) development of a kinetic model of the transformation on a modified MgO-SiO2 catalyst and estimation of its parameters using published data; (iv) highlighting of some interesting peculiarities of the transformation at the level of the porous catalyst grain, the most important being the occurrence of a maximum in the dependence of the average speed of BD formation in the grain, in relation to its diameter. This shows that the size of the catalyst particle is an important parameter of the reactor design, in the case of complex chemical processes; (v) a comparative evaluation, by mathematical modeling and simulation, of the fixed-bed catalytic reactors performances, in achieving ethanol to BD transformation. This highlighted the superiority of the multi-tubular reactor over the adiabatic multiple bed reactor with heating of the mixture between the beds; (vi) formulating and solving few optimization problems of fixed-bed reactors converting ethanol into BD. The originality of the results is proven by their publication in four scientific articles, in the field of chemical engineering.