The research of the Cyclohexane Oxidation Process Using Methods of Engineering Analysis

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Abstract – The expediency of analysis and generalization of the liquid-phase cyclohexane oxidation regularities by simulation methods on the CAD software complexes have been shown.

Key words – CAD, engineering analysis, simulation, oxidation, cyclohexane.

I. Introduction

In modern scientific studies are widely used computer-aided design and simulation (CAD), which can count technological devices create their simulation models and analyze manufacturing processes that take place in them at all stages (modes) of the plant, to determine operating parameters with less cost of resources, time and means, and while increasing the accuracy of the results.

Computer simulation is widely used for a variety of engineering problems and is based on using the principles of numerical modeling and parallel experimental analysis of object for the purpose of verifying of the received data. The advantages of this method are a significant resource saving, accuracy and speed of calculations, the ability of prediction and optimization the technical and economic parameters of various processes [1].

II. Scientific aspects

The cyclohexane (CHX) oxidation process to cyclohexanol (COL) and cyclohexanone (CON) is an important industrial process. Its aim products (AP) are used as original products for synthesis of the polyamide fibers – nylon and capron [2]. This process, like a most liquid-phase hydrocarbons oxidation processes with oxygen air (or molecular oxygen), is characterized by low selectivity for aim products and low feedstock conversion: $S_{AP} \approx 78\%$, $X_{CHX} \approx 4\%$ [2].

In the oxidation of higher conversions, there is a sharp decrease in selectivity performances – due to accumulation by-products in the oxidate, especially acids and esters. In turn, low conversion X also makes significant energy costs on the cyclohexane recycling [3].

There are several different methods of intensification of the cyclohexane oxidation, that allow to affect on the speed of realization process, aim products selectivity and their composition [2]. The ratio of the [COL]/[CON] takes an important role in choosing the direction of application of the process: for the high process ratio [COL]/[CON] can be used in the production of adipic acid, and for the low ratio – in the production of caprolactam.

An important contribution to the studying of the cyclohexane oxidation intensification problem have been made by scientists of Lviv Polytechic National University [3-9]. Their researches of the binary catalytic systems and catalytic solutions created by them, on the basis of variable valence metal salt (VVM), in particular the industrial process catalyst – cobalt naphthenate (CoNph) and the organic additives of different nature, testify the positive changes in the technical and economic parameters of the liquid-phase cyclohexane oxidation [3-9]. Recent researches of the developed catalysts action effect indicate the prospects of further researches in this direction [10].

At the same time, the existing results of experimental researches are advisable to analyze and to compile using the simulation methods in the program complexes of computer aided design systems.

Earlier the liquid-phase oxidation has been investigated from the point of view of the chemical kinetics. There were no investigations of hydrodynamics and mass transfer processes in cyclohexane oxidation, though it has a significant influence on the technical and economic parameters. This analysis could be helpful in predicting of the new catalytic systems creation and determining the optimal conditions of the process.

III. Model of the laboratory device

For experimental investigations the compact laboratory reactor has been used [3]. This is the reactor of ideal blending of the bubbling type. The reactor made of steel Ch18N9T (Fig.1, a, b).

a

b

Fig. 1. The laboratory reactor of the bubbling type

For the analysis of chemical kinetics process, hydrodynamics and mass transfer processes of the cyclohexane oxidation we have created a solid model of the laboratory reactor in the CAD software complex SolidWorks 2016 Educational Edition (Fig.2).

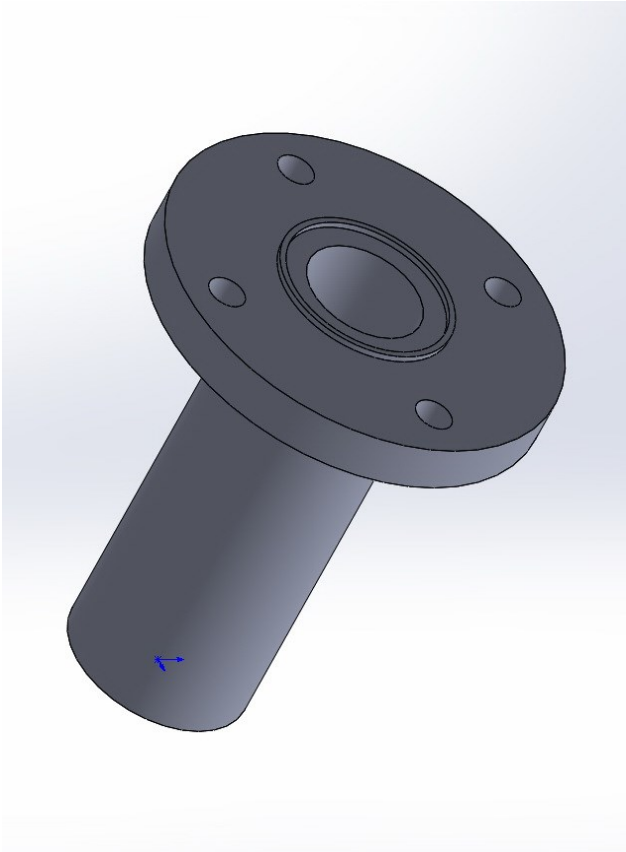

Fig. 2. The solid model of the laboratory reactor in SolidWorks 2016 Educational Edition

Conclusions

The research results will be published. The obtained data can be used for the generalization the existing experimental research, for the creation of new catalytic systems, and as well as for optimization of the process parameters.

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