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OPTIMIZATION OF REACTANT MIXING IN BENZENE ALKYLATION TECHNOLOGY

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Abstract

In this paper the feasibility of mixing device reconstruction in benzene with ethylene alkylation in the presence of liquid-phase catalyst was evaluated using Comsol Multiphysics software. The hydrodynamic model of mixer chamber was developed and optimal options for reactants input are considered. In defined optimal variant a uniform profile of reagents concentration distribution is obtained. The mixing intensification will allow to perform alkylation more effective and reduce catalytic complex flow rate.

Keywords: alkylation; ethylbenzene; mathematical modeling; mixing.

1. Introduction

One of the most progressively developing petrochemicals areas is the production of ethylbenzene - intermediate product required for styrene production [1].

Currently in ethylbenzene production there are a number of problems. For example the presence of concomitant side reactions, due to the presence of undesirable impurities in raw, makes it necessary to improve the selectivity of the process according to the product quality.

The use of acid catalysts leads to equipment corrosion, and high danger of such production requires strict adherence to technological regulations. At the same time, the high cost of reconstruction (the changeover of acid on solid catalysts [2-3]) often is not advisable.

The main urgent problem in ethylbenzene production using aluminum chloride, is the formation of large number of wastewater contaminated by aluminum cations. Aluminum cation concentration in the wastewater is 5 - 15 g/L, during the normal is 0.5 mg/L. Today the problem of chemical-technological systems optimization in general is successfully solved using the hydrodynamic and mathematical modeling methods [4-10].

The purpose of this work is to evaluate the feasibility of mixing device reconstruction of one of the Russian petrochemical plants for the ethylbenzene yield increasing in benzene with ethylene alkylation in the presence of aluminum chloride due to the mixing intensification.

2. Eperimental

Solving the problem of aluminum cations concentration reducing in wastewater can be accomplished by equipment reconstruction for the mixing process intensifying, which will allow to proceed alkylation reaction efficiently and reduce catalytic complex flow.

Using Comsol Multiphysics [9] hydrodynamic model of the mixing chamber (Fig. 1) in which elements are in the form of curved plates was developed, and analyzed for optimal reactants input. Constructive parameters of the mixing chamber are shown in Table 1.

First physical and chemical properties of the substances to be mixed, in particular ethylene, benzene, recycled and fresh catalytic complexes were set (Table 2).

Hydrodynamic modeling was carried out at 333 K and 0.5 MPa, which corresponds to the mixing chamber operating parameters.

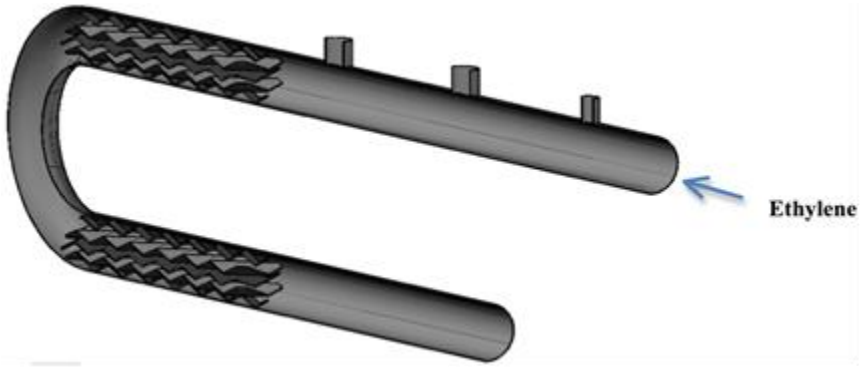

Figure 1. Model of the mixing chamber in longitudinal section

Table 1. Constructive parameters of the mixing chamber

Parameter	Value, m
The length of pipe section	2
The diameter of pipe	0.15
The diameter of pipe branch for dry benzene input	0.08
The diameter of pipe branch for recycled catalytic complex input	0.08
The diameter of pipe branch for fresh catalytic complex input	0.05
The diameter of the mixing element	0.15

Table 2. Physico-chemical properties of the feed streams

Property	Dimension	Benzene	Catalytic complex	Recycled catalytic complex	Ethylene
Molecular weight	kg/mol	0.0781	0.4095	0.024	0.024
Density	kg/m3	845	997	1055	5
Viscosity	kg/(m·sec)	0.0006	0.001	1.04·10—5	1.04·10—5
Flow rate	kg/h	13968	1998	7992	1199
Linear velocity	m/sec	0.914	0.298	0.419	3.77

3. Results and discussion

One of the objectives was the need to determine which of the pipe branches is better to use for the benzene input and which one is for the recycled catalytic complex.

3.1. Determination of effectiveness of pipe branches for the input of recycled catalytic complex and benzene

At the first option it was considered to fed benzene into the second in the direction of ethylene pipe branch, and recycled catalytic complex into the third. The results are presented in the form of color schemes. Color chart in Fig. 2 shows the value of ethylene volume fraction at the first option of components input.

As seen in Fig. 2 the upper mixing element during the reactants mixing is not fully involved in mixing. With such supply of reagents at the outlet of the mixing equipment the flow separation is observed, the volume fraction of ethylene ranges from 0.86 to 0.91.

At the second option, it was considered to fed recycled catalytic complex into the second in the direction of ethylene pipe branch, and benzene into the third (Fig. 3).

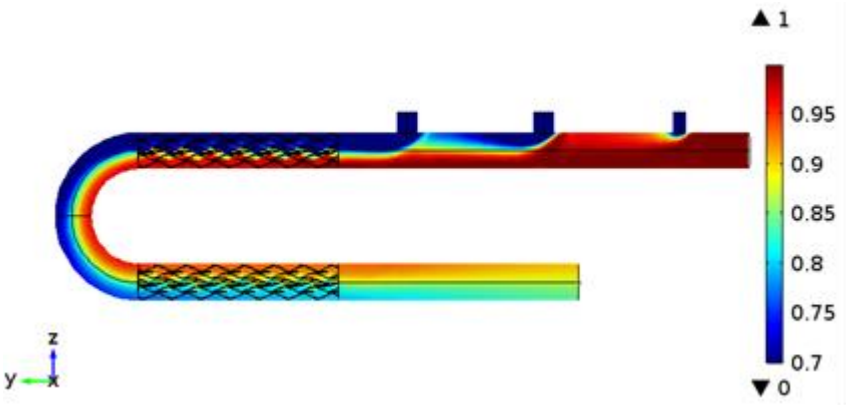

Figure 2. Volume fraction of ethylene at first option (t = 2 sec)

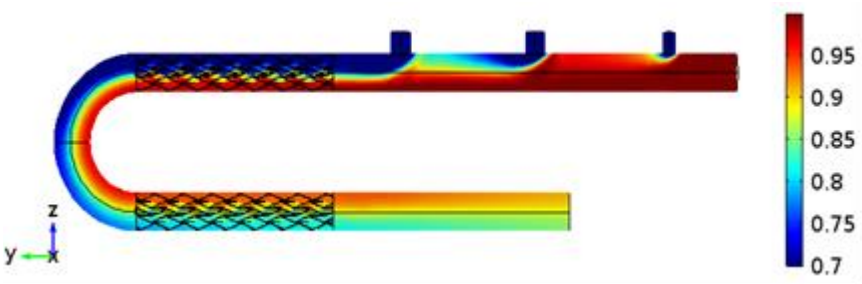

Figure 3. Volume fraction of ethylene at second option (t = 2 sec)

In Fig. 3, similar to the first option of input flow separation at the outlet of the mixing device is observed; the upper mixing element is also not fully used. The volume fraction of ethylene in this case is ranged from 0.86 to 0.93.

3.2. Modification of pipe branches position in mixing chamber

To determine the optimal variant of the intensification process the possibility of pipe branches position modification was considered.

At the third option, it was considered to feed benzene into the first in the direction of ethylene pipe branch, and recycled catalytic complex into the second respectively (Fig. 4).

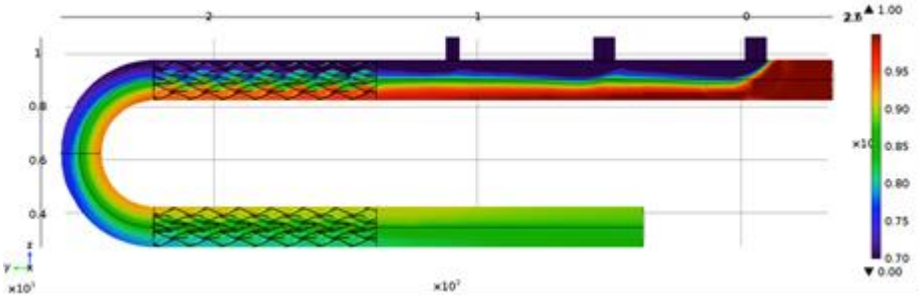

Figure 4. Volume fraction of ethylene at third option (t = 2 sec)

As a result of numerical studies it was defined that such reagents input effects more intensive mixing of the reactants. As seen from the profile the upper mixing element is greater involved in mixing than at others input options. Right after passing through the second mixing element even distribution of the reactants in the bottom part of the mixing chamber is observed: volume fraction of ethylene is set at 0.89.

4. Conclusions

At this point, with the use of Comsol Multiphysics software the hydrodynamic modeling of the mixing device in liquid phase benzene with ethylene alkylation was determined by reagents input option, in which an optimal component mixing is defined.

Further studies will assess the possibility of the recycled catalytic complex rate reduction in considered technology. Reducing of catalytic complex rate, in turn, will reduce the aluminum cations content in wastewater.

Acknowledgements

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