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Procedia Chemistry 10 (2014) 297 – 304

Procedia Chemistry

XV International Scientific Conference "Chemistry and Chemical Engineering in XXI century" dedicated to Professor L.P. Kulyov

Hydrodynamics of reactant mixing in benzene with ethylene alkylation

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Abstract

The purpose of this work is to numerically research benzene alkylation with ethylene over $AlCl_3$ catalyst and assess a feasibility of the alkylation reactor mixing equipment reconstruction using methods of computational fluid dynamics. To evaluate the effectiveness, a simulation of the mixing chamber was developed using ABAQUS and FlowVision software systems. It allows solving the problems in fluid dynamics modelling of liquid and gas flows mixing. Different options of reactant input were considered.

Peer-review under responsibility of Tomsk Polytechnic University

Keywords: Alkylation, ethylbenzene, FlowVision, model, mixing chamber.

1. Introduction

Nowadays the production of ethylbenzene plays one of the main roles in petrochemical synthesis. Ethylbenzene is widely used in petrochemical industry as intermediate in obtaining styrene or as feed for production of polystyrene, ABS plastics, and synthetic rubbers. Currently, the world production of ethylbenzene capacity amounts up to 45 million tons per year.

While using ethylbenzene unit with aluminum chloride catalyst, corrosion of equipment, a large amount of aluminum cations, and contaminated wastewater are topical issues. To solve these problems, the used equipment should be reconstructed to intensify the mixing process. As a result it will lead to a more efficient alkylation reaction and reduction of catalyst complex flowrate[1].

Reconstruction of existing alkylation units for modern ones with solid catalysts (eg, zeolites) is not economically feasible due to its high cost[2]. Thus, nowadays improving the efficiency is the main problem of existing alkylation units of petrochemical plants.

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Peer-review under responsibility of Tomsk Polytechnic University
doi:10.1016/j.proche.2014.10.050

Earlier, a mathematical model of benzene with ethylene alkylation was developed in Tomsk Polytechnic University. It allows studying industrial technology numerically[3-5]. However, the study of hydrodynamic processes, namely research of reagents mixing is not possible without the use of modern computational fluid dynamics techniques.

Numerical hydrodynamics research of the mixing process with the use of computational fluid dynamics methods allows studying the feasibility of the mixing equipment reconstruction of the ethylbenzene reactor block, and making recommendations about optimal design of the unit.

Thus, the purpose of this work is to numerically research benzene alkylation with ethylene and assess a feasibility of the alkylation reactor mixing equipment reconstruction using methods of computational fluid dynamics.

2. Simulation of reactants mixing in benzene with ethylene alkylation

In the majority of operating Russian industrial plants of ethylbenzene production, the mixing of reactants with catalyst complex is as follows: the first stage is mixing of fresh and regenerated catalyst in a chamber upstream of the reactor, and the next stage is feeding of the stream into the alkylation reactor equipped with ethylene gas bubbling device. But, unfortunately, this scheme is inefficient, so additional mixing elements are used to intensify this process.

Reconstruction of the mixing chamber involves its retrofitting with new mixing devices «Sulzer» - metal rods, set directly in the mixing chamber. To evaluate the effectiveness of the mixing device «Sulzer» for the ethylbenzene production, this mixer was simulated using ABAQUS and FlowVision software systems (Fig. 1).[6,7]

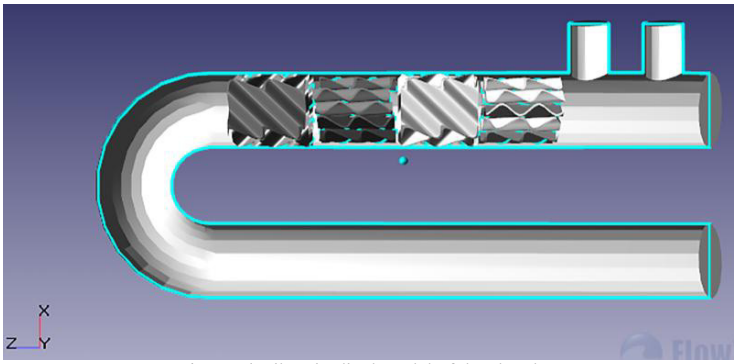

Fig. 1. The llongitudinal model of the chamber

2.1. Determination of the effective pipe nipple use

The main problem was to determine one of the pipe nipples which is better to use for benzene input, and one for catalytic complex input[8,9]. Therefore, the calculations were performed for two options of benzene and catalyst inputs: a) input through the pipe nipple sequentially, in the left - the catalyst, in the right - benzene; b) reverse input. The results of the solution are presented in the color schemes. The color scale in the figure represents the numerical value of the mass or mole fraction.

- Input of benzene in the right pipe nipple and catalyst in the left pipe nipple

As it can be seen from Fig. 2, good mixing of flows is observed after the second mixing element, the mole fraction of benzene at the outlet of the chamber is 0.7-0.8.

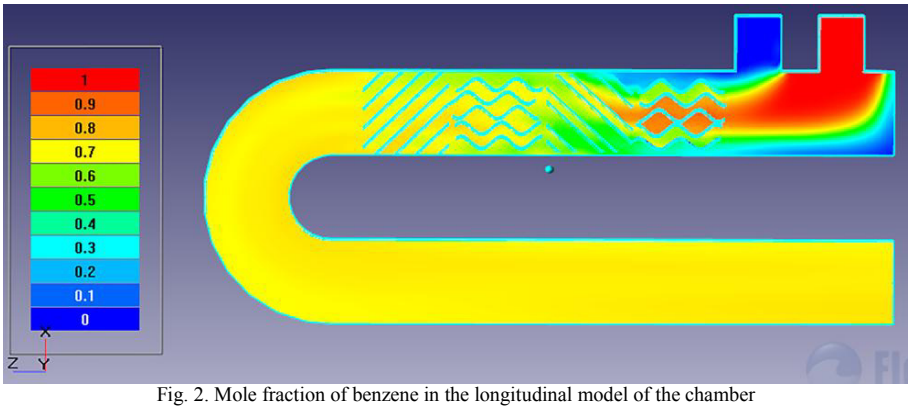

Fig. 2. Mole fraction of benzene in the longitudinal model of the chamber

The mole fraction of the catalyst at the outlet of the pipe is 0.1-0.15 (Fig. 3), the physical properties of substances that enter the chamber explain the structure of outlet flow. Due to the high density and high molar mass, the catalyst is located at the bottom wall of the chamber, then the layer of benzene is located, and at the top, in cross section, there is a maximum molar fraction of ethylene.

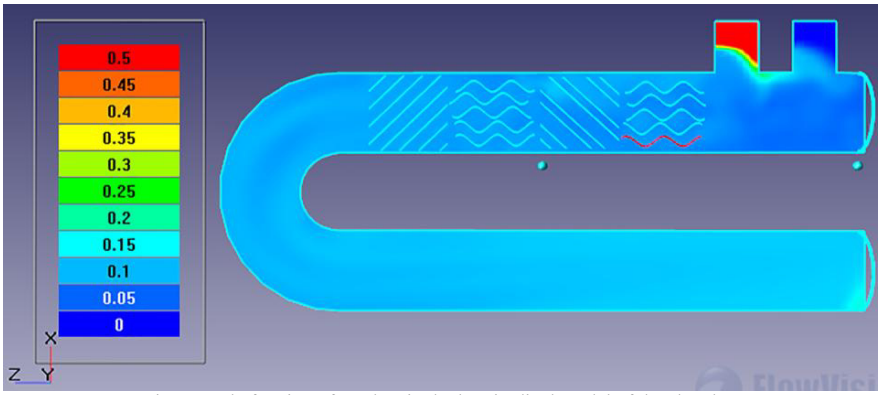

Fig. 3. Mole fraction of catalyst in the longitudinal model of the chamber

Speed of the process determines the total surface area of gas bubbles, that is why homogenized gas distribution over the entire model has a positive impact on the process (Fig. 4).

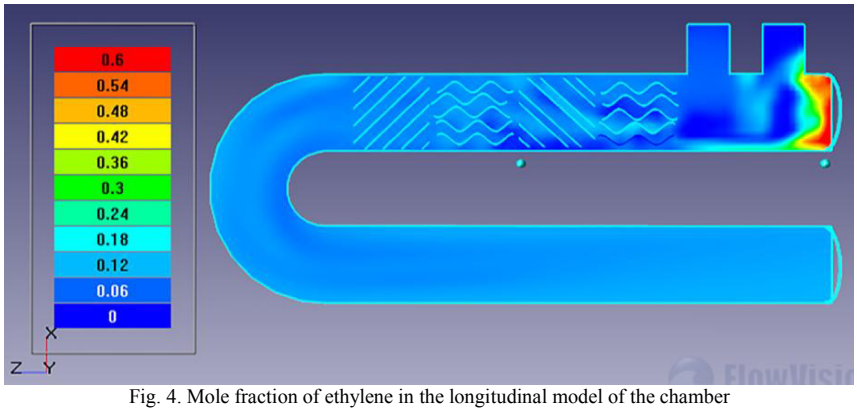

Fig. 4. Mole fraction of ethylene in the longitudinal model of the chamber

Colour schemes show that in this option of the reactant inlet, mole fraction of benzene is 0.7-0.8 at the outlet, mole fraction of catalyst is 0.06-0.15, and mole fraction of ethylene is 0.06-0.12.

- Input of catalyst in the right pipe nipple and benzene in the left pipe nipple

In this option output mole fraction (0.8-0.9) is higher than in the first option at the input of the mixer. The flow structure is much less homogeneous than in the first option.

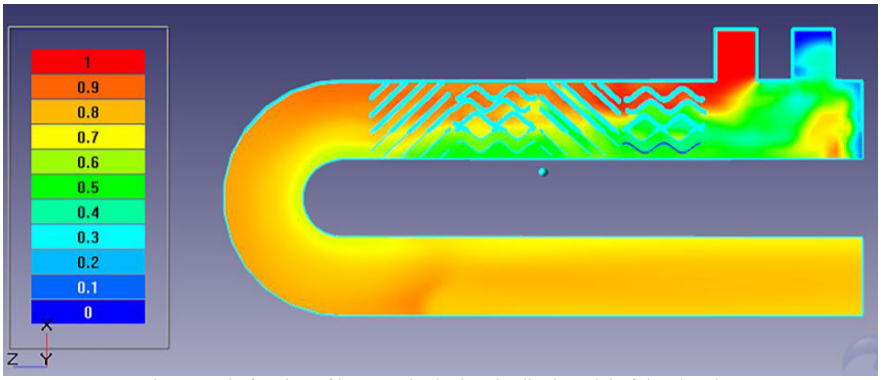

Fig. 5. Mole fraction of benzene in the longitudinal model of the chamber

The mole fraction of catalyst in the chamber is 0.06-0.08 that is lower than in the first option.

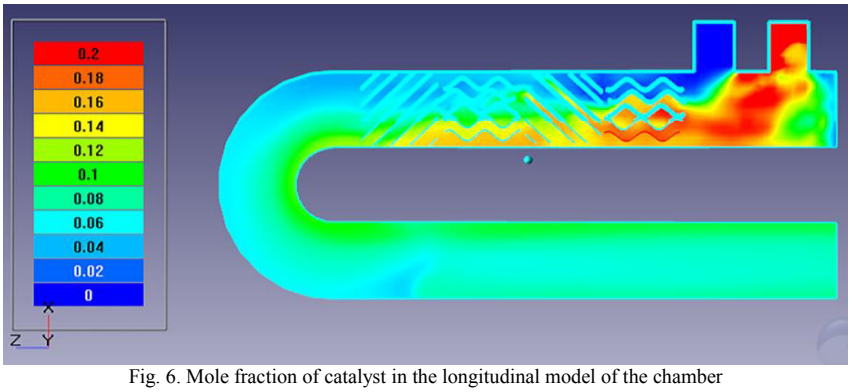

Fig. 6. Mole fraction of catalyst in the longitudinal model of the chamber

The catalyst in this option of the input is distributed unevenly in the cross section of the chamber. There is less relative gradient of concentration in the first option (Fig.7).

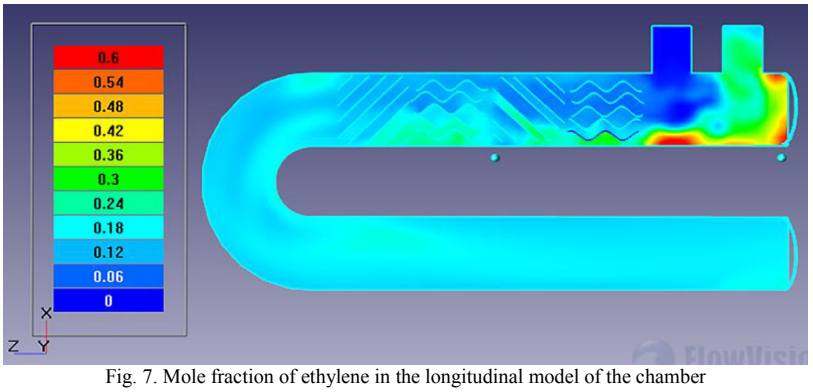

Fig. 7. Mole fraction of ethylene in the longitudinal model of the chamber

In this option, the reactant input presents homogeneous distribution of ethylene throughout the longitudinal model of the chamber, the mole fraction of ethylene varies in the range 0.06-0.18.

2.2. Use of additional mixing equipment

In this process, at the stage of reagents mixing by supplying ethylene to the chamber, the alkylation reaction proceeds; however, to increase the reaction rate as well as to homogenize the structure of the reactant mixture, it is necessary to increase the surface area of interaction[10]. This can be achieved by applying the additional mixing equipment.

This paper describes the installation of disks at the entrance of the mixing chamber. These disks can change the structure of ethylene flow at entrance.

- Installation of the disk with one hole

Mole fraction of the catalyst in the longitudinal model of the unit was 0.05 (Fig. 8), the catalyst is evenly distributed throughout the cross section of the chamber. The concentration gradient does not occur, and homogenization of the mixture is observed after the third mixing element.

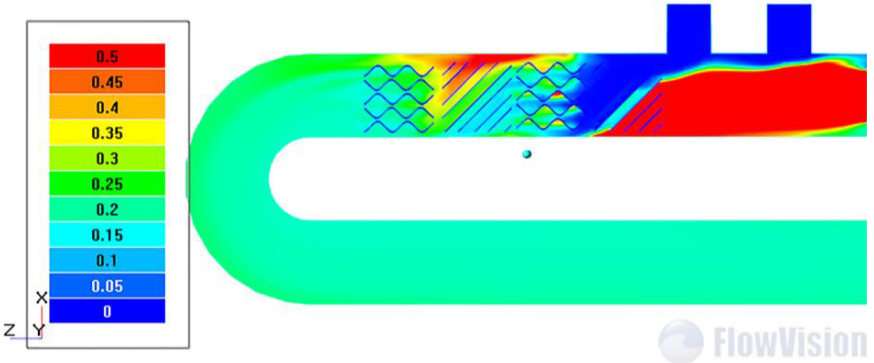

Fig. 8. Mole fraction of ethylene in the longitudinal model of the chamber

- Installation of the disk with two holes

For the mole fraction of ethylene a narrow range of mole fractions was chosen. In this option with two holes, there is a bundle of ethylene flow across the section of the chamber; the structure is less homogeneous than in the first case (Fig. 9).

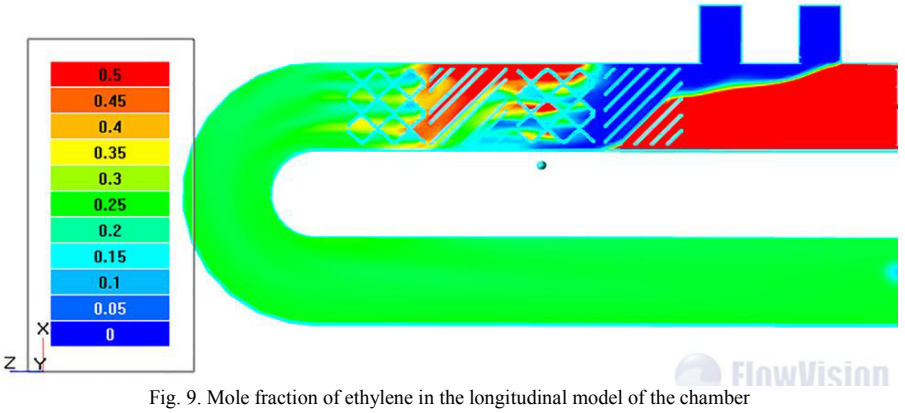

Fig. 9. Mole fraction of ethylene in the longitudinal model of the chamber

- Installation of the disk with three holes

At the outlet of the chamber, the mole fraction of ethylene was 0.2-0.3, the flow structure was even less homogeneous than for the options discussed above. A similar pattern was also observed for the catalyst and benzene.

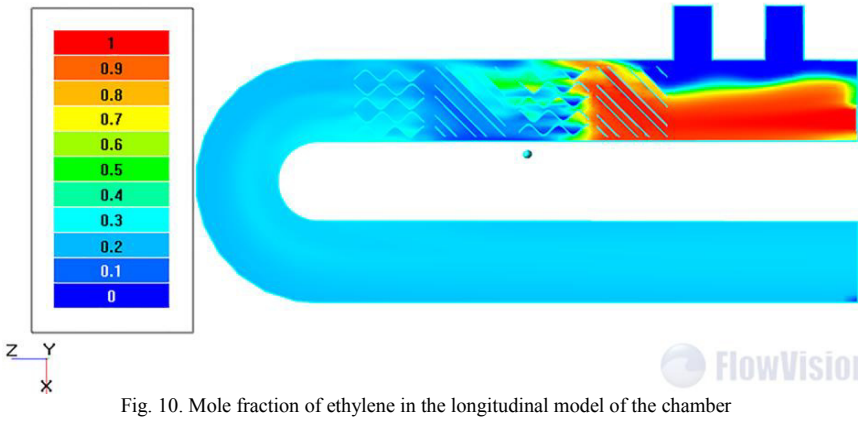

Fig. 10. Mole fraction of ethylene in the longitudinal model of the chamber

The table 1 shows the change of benzene concentration for different inputs in relative %. This rate of concentration change allows assessing an impact of different distributions on yield of the product.

Table 1. Change of benzene concentration for different inputs in relative %

Input of benzene in the right pipe nipple and catalyst in the left pipe nipple	Input of catalyst in the right pipe nipple and benzene in the left pipe nipple	Installation of the disk with one hole	Installation of the disk with two holes	Installation of the disk with three holes
7.09	21.28	2.96	7.41	11.85

As it can be seen from the Table 1, the best option is the installation of the disk with one hole and the option of benzene input in the right pipe nipple and input of catalyst in the left pipe nipple.

The results of calculations allowed determining a general lack of considered equipment - the presence of "dead zones", i.e. places in the chamber, in which the reactants (ethylene and catalyst) don't move.

In spite of the revealed lack, the mixing was significantly improved.

3. Conclusion

The calculations demonstrate that the mixing chamber reconstruction of benzene alkylation with ethylene reactor block will intensify alkylation process. It was concluded that it is preferable to use the right pipe nipple for the catalyst input and the left pipe nipple – for benzene input, because in this case the maximum output of benzene concentration and its uniform distribution throughout the sectional pipe area are obtained.

It was revealed that the use of additional elements (disks with holes) in the mixing chamber, on the one hand, leads to the formation of "dead zones". But, on the other hand, due to the disks, a high degree of reactants mixing is achieved that may be proved by low concentration gradient in the cross section of the mixing chamber.

Acknowledgements

Work is performed as a part of the state Russian Government Project "Science" 1.1348.2014.

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