«Computational Fluid Dynamics Modeling of Mixing Process for Two-Components Mixture in the Large Scale Reactor»

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***Abstract* – The CFD modeling of mixing process of the two-component reaction mixture in a large scale reactor was performed. The modeling results can be used in the following studies to develop real industrial designs of the apparatus.**

***Keywords* –mixing process, large scale vessel, computational fluid dynamics, numerical modeling, mesh density.**

Introduction

There are a lot of industrial processes in chemical engineering where mixing plays a critical role in different applications. Among them are homogenization, suspension, dispersion, heat and mass transfer, temperature uniformity, etc. The most common mixing process is the mechanical type provided by mechanical agitators with a different design.

For the chemical industry, the topic of mixing is especially of interest, since it is a common unit operation in many processes and empirical and semi-empirical correlations for predicting the hydrodynamic characteristics inside a batch mixing vessel do not consider the complete three-dimensional geometry of the vessel and impeller. This is important in processes such as crystallization, dissolution, compounding, and cellular production in bioreactors and others, and the obtained information can aid in the selection of the mixer geometry, the choice of mixing speed and for achieving comparable scale-up/down operation of laboratory and industrial mixing vessels.

Recently, Computational Fluid Dynamics (CFD) techniques have been widely used to reduce the investments and operating costs to analyze and optimize agitators' design and other equipment in chemical engineering. [1-3]. Simulations offer the possibility to obtain a deeper understanding of the evaluated process and can provide information that cannot be easily measured. Furthermore, CFD simulations consider the complete three-dimensional geometry as opposed to more basic correlations and various operational conditions and vessel/mixer geometries can be tested without the need for laboratory and large-scale operation.

In addition, CFD has been widely used to simulate mixing processes due to a lot of agitators configurations and its influence on the properties of the blend or on the process parameters that can be simulated in a short time.

In other words, using CFD requires consideration of many theoretical aspects of the mixing process. First of all, the computational mesh must fit all internal vessel elements, vessels wall contours and agitators blade. Next, the mathematical model should describe in detail the hydrodynamics and physical properties of fluid for a qualitative evaluation of the mixing process.

In this research, as the modeling object has been selected the large-type vessel to reflect the influence of different simulation parameters and their evaluation on the modeling results and the flow field behavior inside the vessels.

Results and Discussion

The agitator which rotates in fluid volume provides fluid by energy, that creates complex circulation flows. The program complex of numerical simulation ANSYS Fluent 16 was used, as an instrument for simulating of the reaction mixture mixing process in the large-scale-reactor. The essence of such an approach, that implemented in ANSYS Fluent, lies in the numerical solution of the basic equations of hydro-dynamics, namely - the equation of continuity, the equation of conservation of the momentum, the energy conservation equation. These equations have expressed a base model of the flow and may be supplemented by equations for modeling turbulence, component transport, chemical reactions, and the like. The RANS approach has been used for turbulence modeling. The basic equations of the model were supplemented by k-w SST turbulence model to model the flow behaviour. The mixture of 2,3-dimethylbutadiene and methylmethacrylate was used to modeling this process.

The model of the large-scale-reactor was created by the means of 3D modeling ANSYS Design Modeler and is presented in Fig. 1.

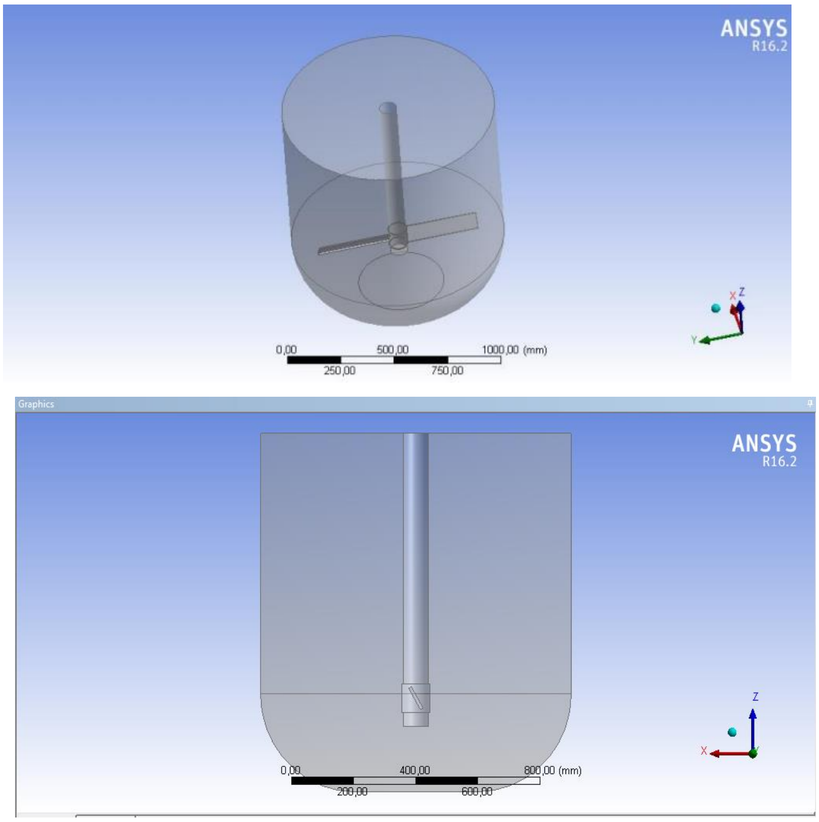

Fig. 1. The reactor geometry

The diameter of the reactor is 1000 mm, the height is 1470 mm. The reactor is equipped with a stirrer, the diameter of the stirrer is 520mm the height is 933mm. The geometric dimensions of the stirrer sketch blade 76/10 mm. The angle of the stirrer blades is 30 degrees. The distance from the bottom of the tank to the stirrer is 375 mm

The mesh model, that was used for simulation, had created in the Mesh preprocessor, which contains approximately 645 300 tetrahedral elements (fig.2). It should be noted, that the greatest density of the mesh is concentrated in the area of the blades, where the highest gradients of speed are observed.

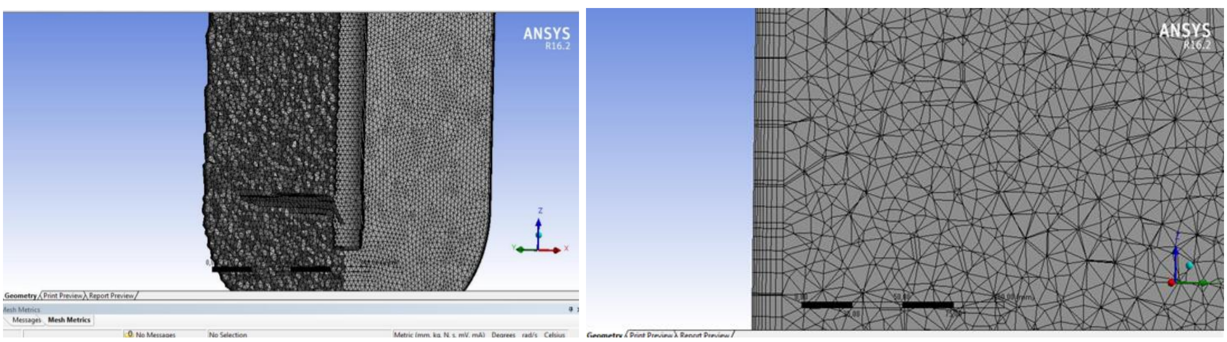

Fig. 2. The mesh of reactor

As results of simulation we obtained the contours of the velocity flow field in vertical cross-section of vessel domain and compared of velocity values in different points of the domain.

According to the presented results, it was installed, that the maximum flow rate is observed in the lower part of the reactor, where the agitator was located. Inside the flow domain there are small-scale local stagnation zones, where zones of zero flow have been formed. The fluid is moving in circular trajectories in the mixer zone. The circulatory flows that will have formed at the top of the reactor are causing an increase in the concentration of the solution in the lower part of the reactor. These observations have been clearly agreeing with the results of experimental research performed earlier.

Conclusion

The computer modeling of the hydrodynamics of the medium in a reactor with a stirrer was performed. A three-dimensional model of components mixture in a large-scale reactor has been developed using computational fluid dynamics techniques. The flow model takes into account the availability of two components mixture and their interactions have based on the the Euler-Euler approach. The modeling results have given an opportunity to draw a conclusion, that the developed model will be using to evaluate the hydrodynamic picture, velocity field, turbulence intensity, determination of mixing power, efficiency of mixer design.

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