

Computational Fluid Dynamics (CFD) Study of Mixing and Heating Time Prediction for Two-Components Mixture in the Small-Scale Reactor

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Abstract – *The CFD model of mixing and heating process of the two-component reaction mixture in a small-scale reactor is presented. The simulated results have been compared with experimental data and given the opportunity to evaluate the application of the proposed approach to the development and design of large-scale apparatus for the synthesis of allyl-1,3,4-trimethylcyclohex-3-enecarboxylate in industrial conditions.*

Keywords – mixing, heating, CFD (Computational fluid dynamics) modeling, sliding mesh, small-scale reactor.

Introduction

The industrial synthesis of many compounds in chemical technology occurs in mixing reactors [1-7]. It is well known, that the hydrodynamics of the mixing has determined the efficiency of the heat and mass transfer of the reaction medium and the kinetics of the chemical reaction. In addition, the physical properties of the original reagents have a strong effect on the efficiency of the process.

In many cases, the mixing is carried out mechanically through having been used various designs of mixers. The experimental research in laboratory conditions which directed at optimizing of the design of stirring mixer device, the geometry of the apparatus, determining the energy consumption for mixing and determining the optimal conditions for conducting of the process, have been often detected ineffective. This is due to the fact, that the energy efficiency and the intensity of mixing are reduced in the transition from laboratory models to industrial plants and at increased the volume of reactive capacity. The holding of the experimental research on an industrial scale is quite expensive and requires considerable time consuming, and in some cases, it may not be feasible at all.

The authors of the study offer being used the methods of computational hydrodynamics, such as an alternative approach. The main advantage of numerical simulation of mixing tasks is the independence from the scale factor. However, one of the main problems arising in numerical simulation of the mixing process is the choice of an adequate model of turbulence and a model that will have been describing the interaction between components of the mixture. With this in mind, it is crucial to verify the results of CFD simulations with the results of a physical experiment to evaluate the mixing process.

Results and Discussion

Mechanical mixing in the reactor volume is a complicated hydrodynamic process that carries out using mechanical stirrers. The mixer which rotates in fluid volume provides fluid by energy, that creates complex circulation flows. Traditionally, the three levels of mixing are distinguished: macroscale, mesoscale and microscale. Each scale is characterized by different vortex structures of streams in the apparatus and has a different nature.

The microscale vortices constantly are changing in size and shape also primarily depending on the pulsating component of the speed, at the same time as the vortex structures of the macro- and mesoscales will have been resistant in size and shape, which respectively complicates the simulation process.

The authors of the study had used the program complex of numerical simulation ANSYS Fluent 17, as an instrument for simulating of the reaction mixture mixing process in the small-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 model of the small-scale-reactor in the form of the internal domain was created by the means of 3D modeling ANSYS Design Modeler and is presented in Fig. 1. The diameter of the reactor is 50 mm, the height is 60 mm. The reactor is equipped with a stirrer in the form of a cylinder (rod) with a diameter of 8 mm and a length of 25 mm. The speed of the mixer is makeup 40 rpm.

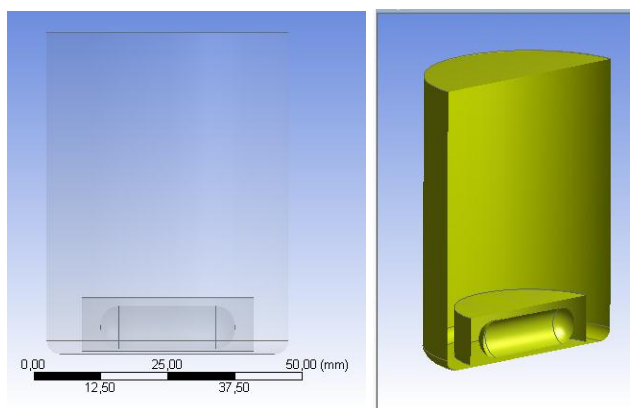


Fig.1. The microreactor geometry

The authors have used the sliding mesh approach Sliding Mesh for correct modeling effects of interaction between elements and zones, that are moving with different speeds in the small-scale-reactor because in this approach the mesh elements of different zones physically are moving one relative to one another. That's why, the geometric scale area calculation was divided into two separate domains - the inner domain (internal moving domain) and the outer domain (outer area). In addition, this approach allows us to simulated the mixing process in the non-stationary formulation, which is extremely important in view of the simulation of the chemical interaction between mixture components.

The mesh model, that was used for simulation, had created in the Mesh preprocessor, which contains approximately 500 thousand unstructured tetrahedral elements. It should be noted, that the greatest density of the mesh is concentrated in the area of the mixer, where the highest gradients of speed are observed and near the reactor wall where the heat flux is dominated.

The RANS approach has been used for turbulence modeling. The basic equations of the model were supplemented by k-e RNG, k-e Realizable and k-w SST turbulence models to model the flow behaviour. The simulation of the components interaction was carried out by means of the model Species, as well as the Euler-Euler approach - the mixture model Mixture. The choice of a mixture model has a significant advantage over other models of the Euler-Euler approach in

practical application. This model is less resource-intensive, and for homogeneous mixtures and systems similar to them it has been more resistant compared to other models. The physical properties of the mixture components (density, viscosity) are presented in table 1.

Table 1

The physical properties of the mixture components		
Compounds	Density, g/cm ³	Viscosity, Pa·s
2,3-dimethylbutadiene	0.726	0.0000727
allylmethacrylate	0.9335	0.0006

In the ANSYS Fluent program was implemented the Species model for the simulation of homogeneous mixtures that consist of several components and effectively mix at the molecular level. This approach has also been used for modeling of the mixture behaviour.

The additional boundary conditions on the walls, method of resolution, sampling schemes, properties of the materials, and so on were set up in the process of setting up the ANSYS Fluent solver.

The results are showing the behaviour of the flow and help explain the physical experiment results. According to the presented results, it was installed, that the maximum flow rate is observed in the lower part of the reactor, where the mixer was located. In the device, 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

A three-dimensional mixing model of components in a small-scale reactor has been developed using computational fluid dynamics techniques. The rotational movement of the mixer has been modeling on the basis of the Sliding Mesh approach.

The flow model takes into account the availability of two different mixture components and their interactions have based on the Species model, as well as the Euler-Euler approach - the Mixture model.

The presented results have given an opportunity to draw a conclusion, that the developed model will be using to predict the time of non-stationary mixing for the purpose of simulation industrial type machines and optimize technological processes for the synthesis of allyl-1,3,4-trimethylcyclohex-3-enecarboxylate.

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