Simulation of the hydrodynamics in polymerizers based on the CFD model for the synthesis of rubbers and plastics using the method of the solution polymerization

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Abstract. Mixing in a viscous medium, such as in polymerization processes, is worth noting. To control the polymerization process for improving the product quality, it is important to understand the mixing process. Also, it is essential to understand the flow behaviour in the stirred-tank reactor for the equipment design and from the point of view of the large-scale transition of the process. Local and general characteristics of mixing in the reactor are related to the design and selected speed of the agitator. 3D-modeling of the flow in the cylindrical reactor with the paddle stirrer was carried out using the potential of a supercomputer. Numerical results showed good consistency with experimental results and correlation developed by other researchers. To determine the best mode of introduction into the paddle space of the stirrer, two efficiency criteria were used: with respect to power and mixing time.

1. Introduction

Earlier research on mixing is based on the development of mathematical models of mixing [1-11]. The problems that occur in these models for periodic or continuous polymerization in the stirred-tank reactor are related to the fact that the increase in viscosity during the polymerization quickly changes the initial assumptions about the homogeneity, which regulate the main aspects of the mixing process. Another problem for the stirred-tank reactors is the difficulty of combining mathematically complex polymerization kinetics with mixing models. These problems can be partially overcome using the computational fluid dynamics (CFD). Computational fluid dynamics is a design tool for developing new processes and optimizing existing ones. The development of computational fluid dynamics has made it possible to visualize mixing processes without conducting the real-time experiments, which are not feasible in some cases. Recent developments in the computer technology have made the computational fluid dynamics an attractive tool for designing, optimizing and visualizing various processes.
es. Mixing models which are implemented using the computational fluid dynamics can be useful in the transition from laboratory installations to industrial production [12-22]. CFD provides the information about the turbulent zone and introducing reagents in areas with the intense turbulence can help improve the product yield.

Radial fluid flows are mainly created in the stirred-tank reactor with turbine agitators. When working with turbine agitators with a large number of revolutions, along with the radial flow, a tangential (circular) flow of the device contents and the formation of a funnel may occur. In this case, the infringement baffles are installed in the device.

2. Materials and Methods
In this paper, the velocity fields in the stirred-tank reactor were studied for a stationary process using ANSYS Fluent.

It is built the geometry of the device with a radius of 0.15 m and a height of 1 m, the agitator radius of 0.05 m, the mixing arm height of 0.022 m, the mixing arm length of 0.04 m, the mixing arm thickness of 0.004 m, the agitator shaft diameter of 0.02 m, the speed of rotation of the agitator varied within 1-20 rpm. Hexane was chosen as the working fluid so it has an absolute viscosity at 20°C of $0.3 \times 10^{-3}$ (dyne·s/cm²) and a density of 655 kg/m³.

The stirred-tank reactor creates a three-dimensional flow, so the basis of the mathematical solution of the problem is a system of differential equations describing the movement in the reactor with the turbine agitator, which are based on the Navier-Stokes equations and the continuity equation of the three-dimensional problem statement. In this system of 4 equations, the 3 components of velocity and pressure are the independent required parameters.

The flow of liquid in the reactor due to the action of the agitator is represented by current lines. In the solution area, the velocity profiles, such as the average axial, tangential and radial velocities, were obtained.

3. Results
As a result of numerical experiments in the stirred-tank reactor with a turbine agitator (figure 1–8), the existence of an axial flow that provides secondary circulation is revealed.

Creating a model (hydrodynamic module) for the synthesis of synthetic rubber (SR) and software implementation was carried out on the basis of the FLUENT 16 software package using the supercomputer complex of the Joint Supercomputer Center of the Russian Academy of Sciences.

Computational fluid dynamics algorithms for an incompressible fluid are based on solving the Navier-Stokes or Reynolds equations (elliptical type) to determine the pressure that connects the entire flow region at each moment of time.

![Figure 1. The network in the sector of the reactor.](image-url)
Figure 2. The field of total velocities in the stirred-tank reactor.

Figure 3. The profile of total velocities in the cross section of the mixing arms.
Figure 4. The radial velocity profile in the cross section of the mixing arms, laminary viscosity model.

Figure 5. The axial velocity profile in the cross section of the mixing arms, viscous laminar model.
Figure 6. The radial velocity profile in the cross section of the agitator arms, k-ε model.

Figure 7. The axial velocity profile in the cross section of the agitator arms, k-ε model.
Figure 8. The total velocity profile in the cross section of the agitator arms, laminar viscosity model.
The implementation of computations of all the main resource-intensive operations leads to the need to parallelize the task on the supercomputer. An increase in the number of computational units for solving the problem leads to "saturation" in which there is no increase in performance (Figure 9). This is due to an increase in the consumption of exchanging information between computing units. Moreover, the larger the size of the computational stack is, the more the number of units can be used for computation on it. The exchange between computing units is limited by the speed of transfer of information. These phenomena are associated with the limitation of the growth of a computer network by Amdahl's law, while the network topology, memory access problems and its optimization difficulties, possible problems in optimizing the MPI parallelization process are important.

Figure 9. The dependence of the computational error on the number of iterations.

In the calculations, such components of the CFD-model as the geometry of the reactor with the paddle stirrer, the computational grid, the boundary conditions and physical properties of materials, the k-ε turbulence model and the parameters of the numerical solution of the system of transport equations were specified.

The equations are written in the cylindrical coordinates. In this system of 4 equations, the independent required parameters are 3 components of velocity and pressure.

The numerical algorithm is based on the final volume method for the unstructured grid. The complexity of numerical algorithms based on the grid methods for the Navier-Stokes and Reynolds equations is the determination of the relationship between the pressure field and the velocity field, which is provided by the continuity equation implemented using the SIMPLE algorithm on aligned grids. The values of the velocity and pressure fields are stored in the same units that is the centers of the control volumes (aligned grids). From the point of view of software implementation, aligned grids are the most economical.

The calculations were performed on different grids using single precision. Calculations were carried out on a grid containing 1 million cells using 50 processors (200 cores) of a supercomputer.
In addition, the calculation and analysis of the technological characteristics of the agitator was carried out. The power criterion $K_N$ was determined by

$$K_N = z_0 \frac{\pi^2}{6} \frac{h_0}{d_m} \left[1 - \left(\frac{r_m}{r_0}\right)^3\right] Re_c^{-1}$$

(1)

where: $z_0$ is the number of agitator arms, $\lambda$ is the resistance coefficient of the central plates, $h_0$ is the height of projection of the arm on the meridional plane, $m$, $r_m$ is the radius of the inner edge of the arm, $m$, $r_0 = 0.5d_m$, $Re_c = \frac{\rho d_m^2 n}{\mu}$ is the centrifugal Reynolds criterion, where $\rho$ is the density of the medium, $kg/m^3$, $n$ is the rotational speed of the agitator, rps, $\mu$ is the dynamic viscosity coefficient of the medium, $Pa\cdot s$, $d_m$ is the diameter of the agitator, $m$.

The power consumed for mixing $N [W]$ was found as follows:

$$N = K_N \rho d_m^5 n^5$$

(2)

where: $n$ is the speed of the agitator, rps or rpm, $\rho$ is the density of the medium, $kg/m^3$, $d_m$ is the diameter of the agitator, $m$.

Also, one of the most important characteristics is the ram effect (or supply) $V_c$, i.e. the volume of liquid flowing to the agitator per unit of time and, thus, $V_c$ determines the circulation of the liquid in the reactor:

$$V_c = \frac{Q}{n d_m^3}$$

(3)

where $Q$ is the volumetric flow rate, $m^3/s$.

4. Discussion

The copolymerization of isobutylene with isoprene proceeds according to the cationic mechanism. Cationic polymerizations are the least studied which is explained by the very high reaction rate that consists of a large number of stages. This reaction is highly exothermic and is carried out at temperatures which are close to the freezing point of the reaction mass (nearly -95$^\circ$C). Maintaining such a low temperature in the reaction zone is necessary to ensure the quality of the produced butyl rubber, i.e. its molecular weight, composition, viscosity. It is known that when the temperature in the reaction zone rises above minus 50$^\circ$C, the rubber of low molecular weight is obtained, which makes it unsuitable for further use. Therefore, to provide the required low temperature in the polymerization zone, the reactor is equipped with 6 heat exchange elements, which are tube bundles with 205 tubes. The reaction medium is cooled with boiling liquid ethylene, which circulates through the tubes of heat exchangers. Also, to intensify the heat transfer process inside the reactor, it is equipped with a high-speed turbine agitator, which has a rotational speed of about 230 rpm.

Optimal for the mixing process is to reduce the consumed power and increase the ram effect (Figure 10).
Figure 10. The dependence of the power $N$ and ram effect $V_c$ on the radius and speed of the agitator under $\lambda = 42$, $Q = 10^{-6}$ m$^3$/s, $h = 0.3$.

5. Conclusion
Thus, it is obtained the results of numerical simulation of the stirred-tank reactor with the turbine agitator in order to analyze the behavior of the power criterion and other characteristics of the process.

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