Article citation info:
WODOŁAŻSKI A. Modelling of slurry hydrodynamics with two-blade impeller in tank reactor. Eksploatacja i Niezawodnosc – Maintenance and Reliability 2014; 16 (4): 533–536.

Artur WODOŁAŻSKI

MODELLING OF SLURRY HYDRODYNAMICS WITH TWO-BLADE IMPELLER IN TANK REACTOR

MODELOWANIE HYDRODYNAMIKI ZAWIESINY W REAKTORZE ZBIORNIKOWYM Z MIESZADŁEM DWUŁOPATKOWYM*

The paper presents computational fluid dynamics (CFD) method to hydrodynamics modelling of slurry in a tank reactor with a mixer. Numerical calculations were performed for two blade impeller. An analysis to obtain a uniform distribution of the solid particles in the whole volume of the slurry reactor has been carried out. Selected results of hydrodynamics simulation suspended solids catalyst CuO/ZnO in paraffin oil were presented respectively. These studies have been designed to determine the velocity and concentration fields of slurry in the reactor. Numerical calculations have been performed for a suspension of different diameter of particles, bulk density in the mixer without baffles. The lack of baffles had to limit the abrasion of solid particulates and improving the better mass transfer between the solid and the liquid phase.

***Keywords**: CFD simulation, particle suspension, stirrer tank reactor.*

W pracy zaprezentowano metodę obliczeniowej mechaniki płynów (CFD) do modelowania hydrodynamiki zawiesiny w reaktorze zbiornikowym z mieszadłem. Obliczenia numeryczne przeprowadzono dla mieszadła dwułopatkowego. Podjęto analizę nad uzyskaniem równomiernego rozkładu cząsteczek stałych zawiesiny w całej objętości reaktora. Zaprezentowano wybrane rezultaty symulacji hydrodynamiki zawiesiny cząstek stałych katalizatora CuO/ZnO w oleju parafinowym. Badania te miały na celu określenia pól prędkości i stężenia zawiesiny w reaktorze. Obliczenia numeryczne przeprowadzono dla zawiesiny o różnej średnicy cząstek, gęstości złoża w mieszalniku bez przegród. Brak przegród miał na celu ograniczenia ścieralności cząstek ciała stałego oraz zapewnienie lepszej wymianie masy pomiędzy fazą stałą a ciekłą.

***Słowa kluczowe**: symulacja CFD, zawiesina cząstek, reaktor zbiornikowy z mieszadłem.*

1. Introduction

Technological process runners in a tank reactor equipped with mechanical stirrer are widely used in unit operations, such as crystallization, dissolution or conduct of chemical reaction in a three-phase system (with the suspended catalyst). In the chemical industry, these are mainly reactions such as methanol synthesis, Fischer-Tropsch, oxidation of p-xylene to terephthalic acid, production of polymers or using suspension polymerization [2,3,5].

The advantage of the suspension system is that the resulting movement of all the particles dispersed throughout the volume of the slurry reactor, as well as the effective elimination thermal or concentration gradients. This results in a high yield of carried out reactions [4].

The hydrodynamics of the slurry reactor with a stirrer can be characterized by experimental measurements or numerical simulations. However, at present it is difficult to measure the concentration profile in the whole volume of the slurry reactor, in particular in the regions of high dissipation of energy [6]. Mathematical description hydrodynamics of slurry preparation is difficult due to interaction between the flow around a rotating agitator and stationary baffle [8]. In other cases the situation may be complicated by additional reactions taking place in the liquid phase presence of a solid catalyst. It also affects other parameters such as size, type and frequency of stirrer speed. An important aspect is to control of slurry temperature, because it allows to maintain strictly isothermal reaction medium.

In the case, where the rate of heat release exceeds the amount of heat that can be removed by cooling the reactor, there is a significant decrease of the reactions productivity and selectivity [4].

One approach to solve problems related to the optimization of the suspension in the tank reactor is a "Computer Fluid Dynamics" (CFD). It allows for a better understanding of the process, its reliability and safety [3]. Hydrodynamics of the two-phase liquid-solid in a tank reactor is still not sufficiently investigated and quantified described [1]. H.Zhang and N.Qi studied phenomenon and hydrodynamics in the slurry reactor with Smith and Rushton turbine [6]. In available literature there is a lack of data describe impact of two blade impeller on hydrodynamics of the suspension.

The aim of the study was to determine the velocity and concentration fields of the suspension in the reactor for different particle diameter and bed density. Also the effect of dynamic pressure on the blades of the stirrer was analyzed. It plays an important role in the analysis of the mixer efficiency in carrying out calculations in structural strength of the blades. The results can be used in a methanol synthesis process to optimize production costs, problems of the catalyst deactivation or in structural-strength calculations for agitator blades.

2. Methodology and modelling object

In this paper to describe the hydrodynamics of two-phase system was used Eulerian–Eulerian model along with a standard of k-ε turbulence model. This model is based on the transport equations for turbulence kinetic energy (k) and its dissipation rate (ε). Phases: liquid and solid are treated as mutually interpenetrating continua, which provide momentum, energy or mass of the component. The continuity equation (1) and momentum (2) for the analyzed system is given below:

(*) Tekst artykułu w polskiej wersji językowej dostępny w elektronicznym wydaniu kwartalnika na stronie ***www.ein.org.pl***

$$\frac{\partial(\alpha_i p_i)}{\partial t} + \nabla(\alpha_i \rho_i \bar{u}_i) = 0 \quad (1)$$

where: $\alpha_i, p_i, \bar{u}_i$ means the volume fraction, density, velocity vector, respectively, by an index i a solid or liquid phase.

$$\frac{\partial(\alpha_i p_i \bar{u}_i)}{\partial t} + \nabla(\alpha_i \rho_i \bar{u}_i \bar{u}_i) = -\alpha_i \nabla \rho_i + \nabla\left(\alpha_i \bar{u}_i \left(\nabla \bar{u}_i + (\nabla \bar{u}_i)^T\right)\right) + \vec{F}_C + \vec{F}_i + \alpha_i \rho_i \vec{g} \quad (2)$$

where: p, μ, g is the pressure, viscosity and gravitational acceleration, *Fc*- centrifugal Corolis force (Ochieng & Onyango, 2008), and *Fi* is interfacial force of interaction of the liquid to solid phase.

The interfacial resistance of component *i* in solid-liquid system is calculated from the following equation [3]:

$$\vec{F}_{is}^{D} = \frac{3}{4} \frac{C_{D,is}}{d_s} \rho_l \alpha_s |\vec{u}_s - u_l| (\vec{u}_s - \vec{u}_l) \quad (3)$$

where C_{Dis}- drag coefficient calculated from the classical Schiller-Naumann model

The turbulent dispersion force $\vec{F}_{is}^{T}$ is calculated by [3] :

$$\vec{F}_{is}^{T} = C_{TD} C_D \frac{\nu_{tl}}{\sigma_{tl}} \left(\frac{\nabla \alpha_s}{\alpha_s} - \frac{\nabla \alpha_l}{\alpha_l} \right) \quad (4)$$

where: C_{TD} – means the ratio of momentum to penetrate interfacial resistance forces, v_{tl} – turbulent viscosity, σ – turbulent Schmidt number, α_i means the volume fraction respectively to liquid and solid phases. The standard of turbulence *k-ε* model is described by the equations:

$$\frac{\partial}{\partial t}(\alpha_l \rho_l k_l) + \nabla(\alpha_l \rho_l \vec{u}_l k_l) = \nabla\left[\alpha_l \left(u_l + \frac{\mu_{tl}}{\sigma_k}\right) \nabla k_l\right] + \alpha_l P_l - \alpha_l P_l - \alpha_l \rho_l \varepsilon_l \quad (5)$$

$$\frac{\partial}{\partial t}(\alpha_l \rho_l \varepsilon_l) + \nabla(\alpha_l \rho_l \vec{u}_l \varepsilon_l) = \nabla\left[\alpha_l \left(u_l + \frac{\mu_{tl}}{\sigma_k}\right) \nabla \varepsilon_l\right] + \alpha_l \frac{\varepsilon_l}{k_l} (C_{\varepsilon 1} p_l - C_{\varepsilon 2} \rho_l \varepsilon_l) \quad (6)$$

where: Cε1, Cε2, σ_k, σ_ε are the parameters of the standard model *k-ε* and are as follows: Cε1=1.44, Cε2=1.9, σ_k =1.0, σ_ε=1.3 [3].

The turbulence of the liquid phase was calculated based on the Sato turbulence model [7].

The turbulence of the solid phase is modelled using a zero-order equation model, where the viscosity of the solid phase turbulence is proportional to the viscosity of the liquid phase:

$$\mu_{ts} = \frac{\rho_s}{\rho_l} \frac{\mu_{tl}}{\sigma_t} \quad (7)$$

where: σ_t is the turbulent Prandtl number binding kinematic viscosity of solid phase μ_{ts} to the kinematic viscosity of the liquid phase μ_{tl}.

The object of the study was the geometry of flat bottomed tank reactor with an own construction two paddle mixer shown in Figure 1, along with the various dimensions in Table 1. Mixer is located at a height h=0.14D from the bottom of the tank. The liquid phase was a paraffin oil suspension and the solid phase of the CuO / ZnO catalyst particles, whose physicochemical properties are shown in Table 2. Numerical grids were generated using the MixSim 2.1.10 module preparatory with multiple system reference MRF (moving reference frame). To determine the unsteady flow during modeling was used

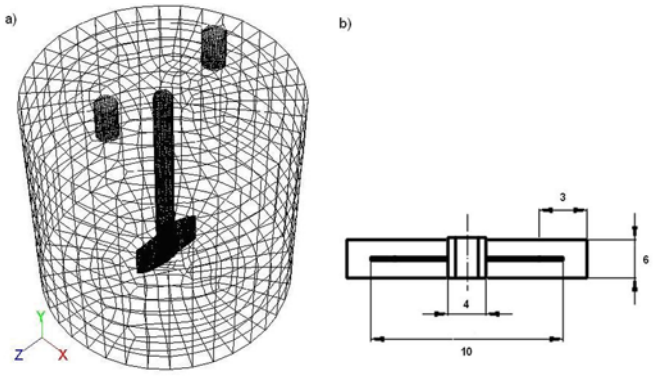

Fig. 1. Stirrer tank model (left- without computing grid), schematic diagram of the impeller-driven stirrer tank (right)

Ansys CFX-12.1 package. The simulation was carried out to time t = 387 s with time step=0,001 s.

The calculation area of the mixing tank was divided into two parts: the inner rotating zone and non-rotating outer zone. In order to improve the consistency and accuracy of the calculation model was made for different mesh densities.

In studies, the following simplifying assumptions were made:
- the tank contains no restrictions of mass transport between the solid and liquid phase
- no slip at the stirring elements and the tank wall
- initial conditions occurs uniformly dispersing the slurry on the bottom tank, while the fluid remains stationary in the remaining part of the tank

Specific parameters of numerical simulation are presented in Table 2.

Table 1. Selected dimensions of the reactor and the parameters of the computational grid

Parameters	Value
Stirrer diameter, mm	15
Height of blades, mm	6
Reactor volume, mm	300
Reactor diameter, mm	49,5
Reactor high, mm	156
Parameters of the numerical grid	
Number of computational cells, thousands	259; 649; 953
The number of cells in the mixer (sliding mesh), thousands	374,350
The maximum skew of grid cells	0,54

Table 2. Main parameters of numerical simulation and physicochemical properties of solid-liquid system

Parameters, unit	Value
The rotational speed of the stirrer, rpm	350-1420
Mixer power, W	4,8-6,5
The density of the catalyst bed, kg/m^3	2000; 4000
The viscosity of a suspension, Pa·s	0,001; 0,002
The size of the catalyst particles, μm	100; 300
The amount of paraffin oil, ml	150
Catalyst loading, (weight %)	0-15

3. Results and discussion

The calculations of velocity field distribution is obtained in a slurry mixer for different stirrer speeds, presented in Fig. 2. Outlines vector of mixing with the visualization of the state of suspension for 47 seconds are shown in Fig. 3. The most intense mixing occurs in the mixer zone, wherein the suspension circulating in the towards to free surface reaching the wall of the tank, next flows towards the bottom of the tank. At low speeds mixer, the dead zones located near the walls of the tank was observed (Fig. 2a). As the increasing rotational speed of the stirrer (890 rpm), followed by properly aligned suspension concentration in the entire reactor volume. In the mixing zone occurs characteristic swirl pattern. Based on the simulation results shown in figures 2 and 4, the hydrodynamics of the slurry in the reactor is mainly dependents on the rotational of the stirrer speed, physicochemical properties of the slurry and loading of the solid phase in suspension.

As a result, calculations of dynamic pressure distributions acting on the blades of the mixer were also carried out (Fig. 3b). The highest dynamic pressure is exerted by the suspension on the blades in their middle part. Also in connection of the rotor blades occur tensions, which must be considered when of the connection design.

Figure 4 shows a normalized distribution of solid concentration of the catalyst CuO / ZnO depending on the density of the bed (Fig. 4a), size of the particles (Fig. 4b). At a time of about 128 sec. and stirrer speed of 890 rpm disperse particles collected from the bottom of the tank are uniformly suspended. Increasing the loading of solid catalyst requires much more mixing power (Fig. 5a). At low rotational speeds, a plurality of instability was observed in the system having a non-uniform dispersion throughout the entire volume of the slurry reactor. Figure 5b shows the distribution profiles of the axial velocity component of the suspension at different loading of the solid phase ($\alpha = 2.5$, 10 % vol. for $\mu = 1 \cdot 10^3$ Pa·s,

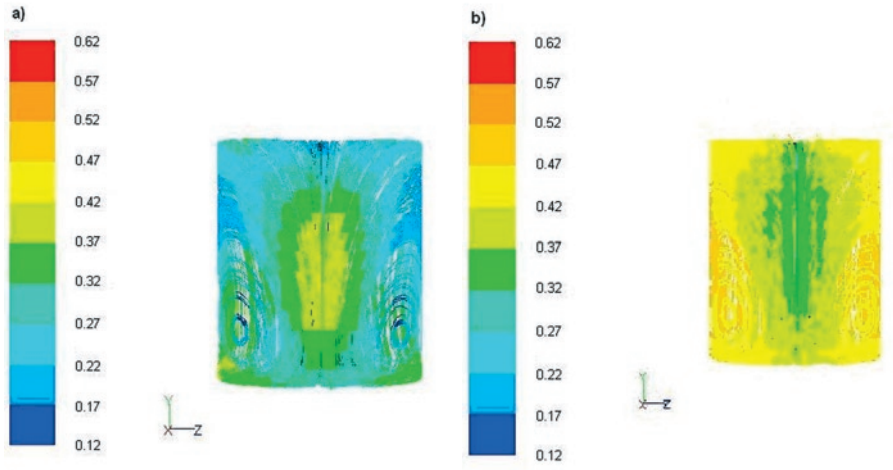

Fig. 2. Contours of velocity suspension in axial plane for selected speed of a stirrer a) 429 rpm, b) 890 rpm

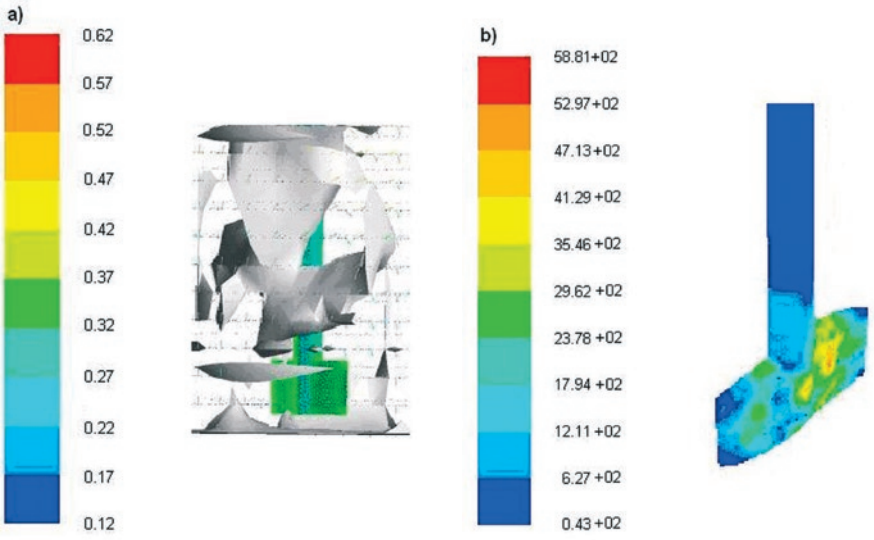

Fig. 3. Velocity vectors of slurry for an axial plane for the stirrer speed 770 rpm (3a), dynamic pressure distribution of the slurry affects on mixer blade, Pa (3b)

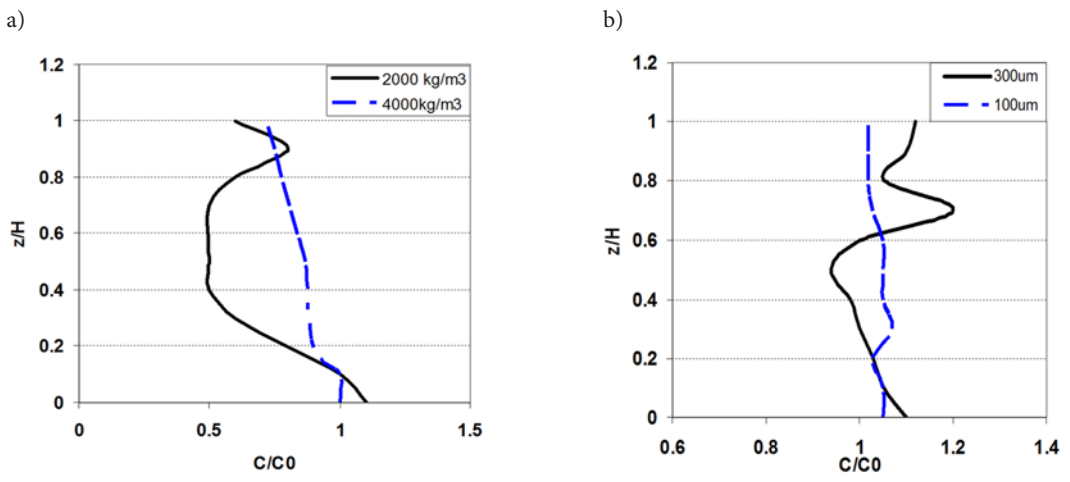

Fig. 4. Normalized distribution of the suspension concentration at the different densities (ρ = 2000, 4000) and the size of the catalyst particles (d_s = 100 μm, 300 μm) for the dimensionless axial coordinate z/H

a) b)

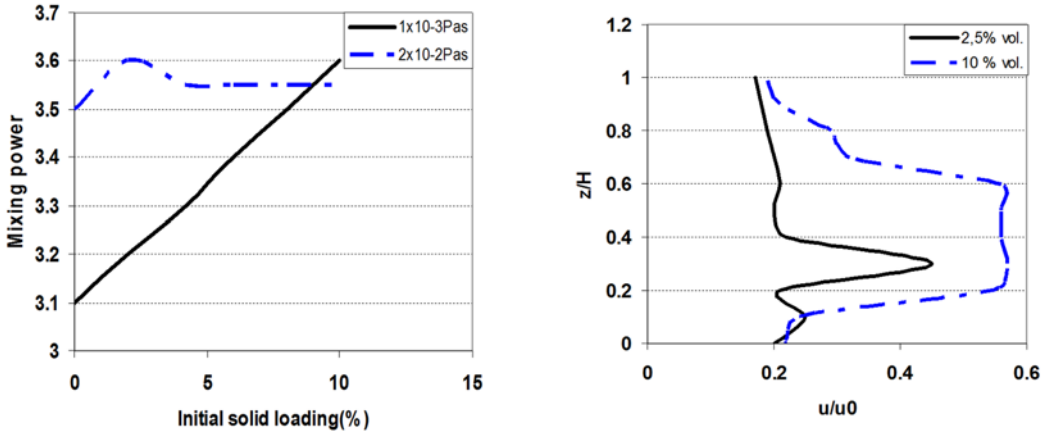

Fig. 5. Mixing power for the different viscosity of the slurry ($\mu = 1 \cdot 10^{-3}$, $2 \cdot 10^{-3}$) at various solid loading (0–10%) for d_s = 100 μm, ρ = 2000 kg/m^3 (5a). Axial velocity distribution of the liquid at selected loading of solid particles (α = 2.5, 10% vol. for $\mu = 1 \cdot 10^{-3}$ Pa·s, ds = 100 um), (5b)

d_s = 100 microns). For the initial solid phase loading of 2.5%, there is a characteristic peak of the axial velocity at the end of the rotor (u_0) where the maximum speed decreases from 0.4 u_0 to 0.2 u_0. Furthermore, the volume of solid phase loading of 10% occurs much greater decrease of the values 0.57u_0 to 0.2u_0, but maintained for a much longer time.

4. Summary and conclusions

In the article was studied the hydrodynamics model of suspension in a two blade stirred reactor. In this simulation Eulerian-Eulerian approach is adopted with a standard k-ε turbulence model. The research leading the following results:

– Power unit number can be predicted for the suspension: liquid-solid through the introduction an average slurry density. For increase initial solid loading of the suspension more power unit number is required for the mixer, and for increased viscosity of $2 \cdot 10^{-3}$ Pa·s, load range of the initial solid phase (0–10%) is maintained at a constant level – Fig. 5a).
– Increase of the suspension density and particle size of the of the initial solid phase increases the descent rate, and also reduces the uniformity of distribution of the solid particles in suspension.
– Higher initial loading of solid particles in the slurry corresponds to the inhomogeneous distribution of the particulate matter in the whole volume of the suspension. Homogenity of the slurry may also be achieved by increasing the viscosity of the solvent.
– Dynamic pressure exerted by the slurry acts on the most front side of the blades.
– Increase of the numerical grid density is significantly longer simulation time, but this allows for considerable precise designation of mixing intensity zones.

References

1. Deglon DA, Meyer CJ. CFD modeling of stirred tanks: Numerical considerations. Minerals Engineering, 2006; 19(10): 1059–1068.
2. Hosseini S, Patel D, Ein-Mozaffari F, Mehrvar M. Study of solid–liquid mixing in agitated tanks through computational fluid dynamics modeling. Industrial & Engineering Chemistry Research 2010; 49(9): 4426–4435.
3. Kasat GR, Khopkar AR, Ranade VV, Pandit AB. CFD simulation of liquid-phase mixing in solid–liquid stirred reactor. Chemical Engineering Science 2008; 63(15): 3877–3885.
4. Montante G, Magelli F. Modelling of solids distribution in stirred tanks: Analysis of simulation strategies and comparison with experimental data. International Journal of Computational Fluid Dynamics 2005; 19(3): 253–262.
5. Murthy BN, Ghadge RS, Joshi JB. CFD simulations of gas–liquid–solid stirred reactor. Prediction of critical impeller speed for solid suspension. Chemical Engineering Science 2007; 62(24): 7184-7195.
6. Qi NN, Wu GY, Wang H, Zhang K, Zhang H. CFD simulation of mixing characteristics in stirred tank by Smith turbine. Journal of Chemical Industry and Engineering (China) 2010; 61(9): 2305–2313.
7. Sato Y, Sadatomi M, Sekoguchi K. Momentum and heat transfer in two-phase bubble flow-I. International Journal of Multiple Flow, 1981; 7(2): 167–177.
8. Yamazaki H, Tojo K, Miyanami K. Concentration profiles of solids suspended in a stirred tank. Powder Technology 1986; 48(3): 205–216.

Artur WODOŁAŻSKI
Central Mining Institute
Department of Energy Saving and Air Protection
Plac Gwarków 1, 40-166 Katowice, Poland
E-mail: awodolazski@gig.katowice.pl