CFD NUMERICAL STUDY OF CATALYST SLURRY HYDRODYNAMICS IN A RUSHTON TURBINE STIRRED TANK REACTOR

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Summary
In this study, three dimensional computational fluid dynamics (CFD) model of catalyst slurry hydrodynamic in Rushton turbine-stirred tank reactor has been developed. The effect of solid catalyst particles distribution in elliptical reactor bottom has been investigated. The numerical calculations have analyzed the effect of catalyst particle size, viscosity and solids loading over a wide range. The results of numerical simulation show that distribution of the slurry concentration depends largely on the stirrer speed and physico-chemical parameters of solid catalyst particles. Effects of catalyst particles cloud height in stirrer tank reactor has been analyzed. Transient analysis of catalyst solid particles volume fraction for different times has been visualized. Dynamic pressure distribution impinge of agitator blades at different stirrer speed were studied. Furthermore, methanol synthesis from syngas derived by coal gasification in this reactor with heat removal option will be carried out.

Keywords: CFD simulation, stirrer tank reactor, catalyst solid particles distribution, Rushton turbine

BADANIA NUMERYCZNE CFD HYDRODYNAMIKI ZAWIESINY KATALIZATORA W REAKTORZE ZBIORNIKOWYM Z TURBINĄ RUSHTONA

Streszczenie
W pracy przestawiono trójwymiarowy model obliczeniowy CFD hydrodynamiki zawiesiny katalizatora w reaktorze zbiornikowym z turbiną Rushtona. Przeanalizowano wpływ rozmieszczenia cząstek stałych katalizatora na eliptycznym dnie reaktora. Obliczenia numeryczne przeprowadzono dla różnych rozmiarów cząstek katalizatora, lepkości oraz załadunku fazy stałej. Wyniki symulacji numerycznej wskazują, że rozkład stężeń zawiesiny w dużym stopniu zależy od prędkości obrotowej mieszadła oraz od fizyko-chemicznych właściwości cząstek stałych katalizatora. Przeanalizowano wysokość chmury cząstek stałych katalizatora w reaktorze. Zwizualizowano ułamki objętościowe frakcji stałej katalizatora dla różnych chwil czasowych w stanie nieustalonym. Określono rozkład ciśnienia dynamicznego oddziaływującego na łopatki przy różnych prędkościach obrotowych mieszadła. W przyszłości w reaktorze zostanie przeprowadzona reakcja syntety metanolu z gazu syntezyowego pochodzącego ze zgazowania węgla wraz z odbiorem ciepła reakcji.

Słowa kluczowe: Symulacja CFD, reaktor zbiornikowy z mieszadłem, dystrybucja cząstek stałych katalizatora, turbina Rushtona

1. INTRODUCTION

Stirred tank reactors are used in the petrochemical and chemical processes taking place in hydrogenation of heterogeneous catalysts such as Fischer-Tropsch synthesis, methanol or polymerization reaction [2,3]. The efficiency of this process depends on the type of the slurry catalyst dispersion in the entire reactor volume. Due to
the type and frequency of stirrer rotation, particle size and the degree of solid loading in the slurry [5]. Solid-liquid mixing systems are used classical two-blade impeller, Smith turbine or six-bladed Rushton turbine [1]. Mixers of this type is characterized by a significantly lower shear stresses affecting the solid catalyst phase, which may lead to its deactivation [6].

A useful tool to study slurry hydrodynamics is CFD (computational fluid dynamics) [8]. It allows to obtain a detailed information of hydrodynamic parameters, as well as to reduce time-consuming and costly experimental measurements, thus minimizing implementation time of the reactor in the technological process [4, 9]. The hydrogenation processes taking place in high temperature and pressure conditions during long-term operation, which can contribute a reduction of reactor service life and process security. Therefore, it is necessary research to led model to defining the strength of impeller blades and hydrodynamics suspension, which allows optimization of the process condition to ensure its effective work in a long period time of industrial exploitation. Numerical modeling of slurry hydrodynamics in tank reactor with Rushton turbine has been analyzed by Yapacity and Wang [7,10]. In the other hand on available literature is the lack of information on the impact of Rushton turbine rotating on the slurry catalyst CuO / ZnO hydrodynamics in the a elliptical bottom reactor.

This paper presents a numerical model of the catalyst slurry hydrodynamics in a elliptical bottom reactor tank with Rushton turbine impeller. The reactor is dedicated for the methanol synthesis from synthesis gas derived from coal gasification in three phase system. The study on the amount of catalyst slurry particle clouds and visualization of shares by volume solids catalyst for different moments of time provides valuable information to determining the relationship between hydrodynamics and process performance, which allows to optimize the operating parameters of the reactor. These simulations allows to assess the quality suspension and determination of the critical frequency of stirrer speed necessary to achieve suspension homogeneity.

Nomenclature

\( \vec{v} \) velocity vector (m/s)
\( u \) velocity (m/s)
\( m_{pq} \) characterizes the mass transfer from phase p to phase q (dimensionless)
\( m_{qp} \) characterizes the mass transfer from phase p to phase q (dimensionless)
\( p \) pressure (Pa)
\( \ddot{g} \) gravitational constant (m/s²)
\( k \) turbulent kinetic energy (J/kg)

\( \tilde{R}_{pq} \) an interaction force between phase p and phase q (N/m²)
\( K_{pq} \) inter-phase momentum exchange coefficient (dimensionless)
\( C_{\mu} \) model parameter constans (dimensionless)
\( C_{1\varepsilon} \) model parameter in turbulent dissipation energy equation (dimensionless)
\( C_{2\varepsilon} \) model parameter in turbulent dissipation energy equation (dimensionless)
\( t \) time (s)

Greek symbols

\( \alpha_q \) volume fraction (dimensionless),
\( \varepsilon \) turbulent energy dissipation rate per unit mass (m²/s³)
\( \mu \) effective viscosity (Pa s)
\( \rho \) density (kg/m³)
\( \tau \) stress-strain tensor of phase q or p (Pa)
\( \eta_0 \) dynamic viscosity (Pa · s)
\( \Omega \) characteristic swirl number (dimensionless)

Subscripts

\( q \) liquid phase
\( p \) solid phase
\( i, j, k \) coordinate axes

2. MATHEMATICAL MODEL

This paper presents a numerical model of slurry hydrodynamics by using the Eulerian–Eulerian two fluid model. Paraffin oil was considered as a continuous phase and catalyst particles as the dispersed phase. The Eulerian-Eulerian approach is adopted to assuming the total average of mass and momentum transfer equations for each phase.

The continuity equation (1) and momentum balance equation (2) for phase q is given by:

\[
\frac{\partial}{\partial t} (\alpha_q \rho_q \vec{v}_q) + \nabla (\alpha_q \rho_q \vec{v}_q \vec{v}_q) = \sum_{p=1}^{n} (m_{pq} - m_{qp}),
\]  \quad (1)

\[
\frac{\partial}{\partial t} (\alpha_q \rho_q \vec{v}_q) + \nabla (\alpha_q \rho_q \vec{v}_q \vec{v}_q) = -\alpha_q \nabla p + \nabla \cdot \tau + \alpha_q \rho_q \vec{g} + \sum_{p=1}^{n} \tilde{R}_{pq} + m_{pq} \vec{v}_p - m_{qp} \vec{v}_q,
\]  \quad (2)
The drag force exerted by the dispersed phase on the continuous phase is calculated as

$$\sum_{p} \bar{F}_{pq} = \sum_{p} K_{pq} (\bar{v}_p - \bar{v}_q), \quad (3)$$

To simulating multiphase flow the RNG (renormalisation group) $k$-$\varepsilon$ model (4) and (5) presented by Yakhot and Orszag(1986) is used in the simulation. This model is much more accurate in predicting the structure of the suspension flow in multi-phase systems with a certain viscosity to simulate turbulent flows rotating in the liquid-solid systems to predicting the rapidly swirling flow.

$$\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho k u_j) = \frac{\partial}{\partial x_j} \left( \alpha_k \mu_{eff} \frac{\partial k}{\partial x_j} \right) - $$

$$\mu_{eff} \frac{\partial u_j}{\partial x_j} - \rho \varepsilon - 2 \rho \varepsilon \frac{k}{\alpha_k}, \quad (4)$$

where:

$$\mu_{eff} \text{ - effective viscosity from equation (6)}$$

$$\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_j} (\rho \varepsilon u_j) = \frac{\partial}{\partial x_j} \left( \alpha_\varepsilon \mu_{eff} \frac{\partial \varepsilon}{\partial x_j} \right) - $$

$$C_{1\varepsilon} \frac{\varepsilon}{k} \frac{\partial u_j}{\partial x_j} - C_{2\varepsilon} \rho \varepsilon^2 \frac{k}{1 + \beta \eta} \frac{\partial k}{\partial x_j}, \quad (5)$$

where:

$$\mu_{eff} = 0.0456, \quad \eta_0 = 4.38, \quad C_{1\varepsilon} = 1.42, \quad C_{2\varepsilon} = 1.68 \text{ are constants for RNG} \ k-\varepsilon \text{ model.}$$

### 3. NUMERICAL DETAILS

A stirrer tank reactor with a Rushton turbine and cooler was employed to carry out the simulation process. Fig. 1a) has shown the general view of reactor geometry. In table 1 we can see the main reactor dimensions. Also, fig. 1b shows impeller invariant dimensions.

#### Table 1. The main reactor dimensions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Impeller diameter, m</td>
<td>0.025</td>
</tr>
<tr>
<td>The blades height, m</td>
<td>0.02</td>
</tr>
<tr>
<td>Reactor diameter, m</td>
<td>0.3</td>
</tr>
<tr>
<td>Reactor height, m</td>
<td>0.72</td>
</tr>
</tbody>
</table>
Table 2. The main simulation parameters and physico-chemical properties of slurry

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stirrer speed, rpm</td>
<td>10-500</td>
</tr>
<tr>
<td>Mixing power, W/m³</td>
<td>4.8-6.5</td>
</tr>
<tr>
<td>Temperature, K</td>
<td>548-623</td>
</tr>
<tr>
<td>Pressure, bar</td>
<td>50</td>
</tr>
<tr>
<td><strong>Physico-chemical properties of slurry</strong></td>
<td></td>
</tr>
<tr>
<td>Density of catalyst bed, kg/m³</td>
<td>3000; 6000</td>
</tr>
<tr>
<td>Viscosity, Pa·s</td>
<td>0.006; 0.05</td>
</tr>
<tr>
<td>Catalyst particle size, µm</td>
<td>200; 400</td>
</tr>
<tr>
<td>Amount of paraffin oil, ml</td>
<td>150</td>
</tr>
<tr>
<td>Catalyst loading, (weight %)</td>
<td>0-10</td>
</tr>
</tbody>
</table>

The numerical solutions of all governing model equations have been obtained for transient behaviour. The 0.01 seconds was chosen as the time step size and 50 iterations were determined as the maximum number of iterations per each time step. The absolute convergence criterion was specified as the residual values of 0.0001. As a discretization scheme was chosen second-order upwind (second row) in order to achieve high accuracy calculations and avoid the phenomenon of numerical diffusion.

4. RESULTS AND DISCUSSION

Unsteady state simulations are carried out for different operation conditions in this study. Fig. 2 has shown the general view of catalyst slurry velocity distributions fields for the selected mixer speed. Increasing rotational speed of the mixer showing the characteristic circulation loop generated by the mixer. A suitable rotational stirrer speed can eliminate the dead zones as evidenced by the differences in vicinity contours of the reactor.

![Fig. 2. The velocity contours of the suspension for the different stirrer speeds a)10 rpm, b) 200 rpm, c) 250 rpm (catalyst particle size ds =200 µm, initial solid loading=5%)](image)

Fig. 3 shows the contours of dynamic pressure distribution acting on the suspension on the blades at different speeds for turbine impeller. These stresses must be taken into account when designing a stirrer, as in conditions of high temperature and pressure blade surface is exposed to erosion caused by collisions of solid catalyst particles.

![Fig. 3. The contours of dynamic pressure suspension distribution impinging on mixer blades for different stirrer speeds a)10 rpm, b) 200 rpm, c) 250 rpm (catalyst particle size ds =200 µm, initial solid loading=5%)](image)
Fig. 4. demonstrate graphically selected cloud height of solid particles for different slurry catalyst volume fraction and impeller rotational speed. The cloud height is an important parameter determining the degree of the suspension homogenisation, which determines its quality. As increasing a volume fraction of solid catalyst particles and impeller rotational speed of the slurry viscosity decreasing. Thus, it is a uniform dispersion of the catalyst slurry particles throughout for the whole reactor volume. At a low concentration of suspension kinetic energy dissipation of the dispersed phase in the continuous phase is significantly reduced as compared to the higher concentrations. Due to the sudden change in the flow field and concentration, a high turbulent fluctuations macroinstabilities forms at the cloud height.

![Fig. 4](image1)

Fig. 4. The cloud height of solid particles in stirred tanks (a) 0.03 volume fraction, 10 rpm (b) 0.5 volume fraction, 100 rpm (c) 0.075 volume fraction, 300 rpm

Fig. 5. shows exemplary visualization contours of the suspension volume fraction for the different time instants. In addition, these results are helpful to determining the catalyst concentration and provide valuable information about the local mass transfer in this type of system, where you can get a specific information about the product, ensuring an adequate contact time of the catalyst particles with synthesis gas.

![Fig. 5](image2)

Fig. 5. The volume fraction contours of the solid catalyst particles for various time intervals (catalyst particle size ds =200 µm, initial solid loading=8%, stirrer speed 200 rpm), respectively a) 10 sec, b) 30 sec, c) 60 sec

Fig. 6. shows normalized distribution of solid catalyst particle concentration at different densities (6a) and particle size (6b). Therefore, suspensions homogeneity increases with the difference in densities between the dispersed and the continuous phase. A larger solid catalyst particles leads to obtain less suspension uniformity and presence a more zones of mixing intensities.
Fig. 6. Normalized distribution a) of the suspension concentration at the different densities ($\rho = 3000, 6000 \text{ kg/m}^3$) and size of solid particles (ds = 400 µm, 200 µm) for the dimensionless axial coordinate z/H.

Fig. 7a) shows the effect of mixing power numbers for the initial catalyst solid loading for the slurry different viscosity. Stirring power increases with increasing the solid loading of the catalyst phase and the viscosity of the suspension. Fig. 7b) shows the mixing time depending on the impeller speed. Actually, the mixing time is defined as the time required to achieve a certain degree of the suspension homogenization. Increase of impeller rotation speed and the size of the catalyst particles increases the time of mixing suspension.

Fig. 7. Model predictions a) mixing power for the different slurry viscosity ($\mu = 5 \times 10^{-2}, 6 \times 10^{-3} \text{ Pas}$) at various solid loading (0-10%); b) effect of rotation impeller speed on the mixing time for different sizes of slurry catalyst particles.

Presented CFD model can capture the essential features of two phase flow field. Flow field agitated by the Rushton turbine impeller can reach homogeneous suspension depends on particle size, bed density and impeller speed. Therefore, bigger circulation loop increase the energy efficiency of turbulent intensity for solid suspension. Obtained simulation result allow for detailed estimation of hydrodynamic parameters influence on slurry quality under various operating condition. Interaction between solid and liquid system influence of catalyst particles mixing time, where mechanism is still unclear.

5. CONCLUSIONS

The article was carried out numerical simulation of copper-zinc catalyst suspension hydrodynamics in elliptical bottom reactor with Rushton turbine mixing impeller. Detailed three dimensional, unsteady state simulations are presented. The research revealed the following conclusions:
- as increase of rotation impeller speed reduced mixing time to achieve a higher degree of suspension homogeneity
- degree of homogenization is a measure of the quality of the slurry, which increases in impeller rotation speed
- dynamic pressure exerted by the catalyst slurry in the mixer blades depends on the impeller rotational speed and pressure acts on impeller front side blades.
- decrease in solid particle catalyst diameter increase degree of slurry homogenization, which may be attained at lower mixer speeds and shorter mixing times.

The results of a numerical simulation regarding the estimates of the hydrodynamic parameters of the catalyst slurry, which are an important in methanol synthesis technology in a three phase system form synthesis gas derived by coal gasification. The efficiency of this process depends on the efficient slurry mixing. It is important both for the project of reactor for industrial scale and the choice of process conditions. The calculation results are the starting point for process optimisation to obtain maximum yield of product per unit reactor volume.

References