Investigation of the influence of heated catalyst feeding system on the intensity of temperature-dependent chemical reaction in the fluidized bed apparatus

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Abstract. A mathematical model was developed and a numerical study of operation parameters of the fluidized bed apparatus for temperature-dependent processes was performed. Fields of catalyst concentration and temperature fields were obtained. The circulation flow analysis was carried out. The effect of the influence of heated catalyst feeder on the efficiency of apparatus heating was analyzed. The change of the circulating gas flows and catalyst structures due to changes in the heated catalyst feeder was shown. The influence of the catalyst fractional composition on the efficiency of apparatus heating was studied.

1. Introduction

Fluidized bed apparatus are widely used in petrochemical industry. Advantages of industrial using of the fluidized bed apparatus are constructive simplicity at elevated heat and mass transfer and mixing of chemical elements in different aggregation states.

There are a lot of works devoted to the design of reactors (e.g. [1]), and also the generalization of models for fluidized bed mathematical simulation (e.g. [2]). Despite the fact that these apparatus are used in the industry for over fifty years, interest in the study of the properties and possibilities of the fluidized bed using is not exhausted. Each structural element contributes to the efficiency of apparatus. The works, considering individual apparatus singularities, regularly appear in recent years. Changes in the character of the movement and concentration of particles along the wall with deflectors are shown in [3]. In [4, 5] the numerical simulation analysis of the cylindrical apparatus projections on the walls influence on the hydrodynamics of the fluidized bed was carried out. Experimental studies with internal elements in a liquid-solid fluidized bed are presented in [6]. Investigations of fluidized bed processes in the column with an inner cylinder were experimentally made in [7]. Modelling and comparative analysis of two large fluidized bed blocks with various gas raw feeders were performed in [8].

In this paper, a mathematical model was developed and a numerical study of the fluidized bed operation parameters of apparatus design for the dehydrogenation of isobutane to isobutylene, passing with the heat absorption, was performed. Catalyst concentration fields and temperature fields were
obtained. The circulation flow analysis was carried out. The influence of structural modifications (changes in the heated catalyst feeder) on the heating efficiency was analyzed. The change of the circulating gas flow and catalyst due to changes of apparatus design was shown. The influence of the catalyst structural composition on the efficiency of apparatus heating, and consequently, on the reaction rate was studied.

2. Problem formulation and solution method

In the present work we study the fluidized bed cylindrical apparatus, designed for reactions with the heat absorption in the presence of a catalyst. In the lower part there is a gas feeder at the temperature of $550 \, ^\circ\text{C}$. There are microspherical catalyst particles with the diameter of 20-200 $\mu\text{m}$ in the apparatus. Along the axis is located a vertical pipe for the feeding of the heated catalyst regenerated at $650 \, ^\circ\text{C}$. In the middle of the reactor, in the working area, are located angular falling through type grids with the free-sectional area of approximately 30% (figure 1, a).

A vertical pipe for the heated catalyst feeding is located in the center of the feeder, as will be shown below, can have a significant impact on the catalyst circulation. Another version of the feeder layout is therefore considered. There is no a vertical pipe in the center. A catalyst feeder simulates a pipe, embedded on the side of the apparatus, and also provides the catalyst flow in the center of the apparatus (figure 1, b).

![Figure 1. Schemes of considered fluidized bed apparatus.](image)

2.1. Fluidized bed model

Continuous multi-phase Euler-Euler model is used in numerical simulations of the fluidized bed. For each of the phases the equations of mass, momentum and energy conservation are implemented. To take into consideration the interaction of particles of solid phases is used an equation that takes into account the change of energy through the change in temperature of the particles. To close the system are used the relationships obtained from the experimental studies of the fluidized bed.

Conservation of mass

$$\frac{\partial \alpha_i \rho_i}{\partial t} + \nabla \cdot (\alpha_i \rho_i \mathbf{v}) = 0,$$

were $\alpha_i$ is the volume fraction of the $i$-th phase, $\rho_i$ is the real density, $\mathbf{v}$ is the velocity.
Conservation of momentum
\[ \frac{\partial \alpha_i \rho_i \mathbf{V}_i}{\partial t} + \nabla \cdot (\alpha_i \rho_i \mathbf{V}_i \mathbf{V}_i) = -\alpha_i \nabla p + \nabla \cdot \mathbf{t}_i + \alpha_i \rho_i \mathbf{g} + \sum_j \mathbf{R}_j, \]  
(2)
where \( p \) is the pressure, \( \mathbf{t}_i = \alpha_i \mu_i (\nabla \mathbf{V}_i + (\nabla \mathbf{V}_i)^T) + \alpha_i (\lambda_i - (2/3) \mu_i) \nabla \cdot \mathbf{V}_i \) is the stress tensor, \( \mu_i, \lambda_i \) are shear and bulk viscosity, \( \mathbf{I} \) is a unity tensor, \( \mathbf{R}_j = K_j (\mathbf{V} - \mathbf{V}_j) \) is the force of interphase interaction.

Conservation of energy
\[ \frac{\partial \alpha_i \rho_i h_i}{\partial t} + \nabla \cdot (\alpha_i \rho_i \mathbf{V}_i h_i) = \alpha_i \frac{\partial p_i}{\partial t} + \mathbf{t}_i : \mathbf{V} + \sum_j Q_{ij}. \]  
(3)
where \( h_i \) is the enthalpy, \( Q_{ij} \) is the heat exchange intensity, \( p_i \) is the solid phase granule pressure.

To account for the interaction of solid phases particles is used an equation that considers the change of energy through a change in temperature of the particles [22]:
\[ \frac{3}{2} \left[ \frac{\partial}{\partial t} (\alpha_i \rho_i \Theta_i) + \nabla \cdot (\alpha_i \rho_i \mathbf{V}_i \Theta_i) \right] = \left( -p_i \mathbf{I} + \mathbf{t}_i \right) : \nabla \mathbf{V} + \nabla \cdot \left( k_{\Theta_i} \nabla \Theta_i \right) - \gamma_{\Theta_i} + \phi_j. \]  
(4)
where \( k_{\Theta_i} \) is the diffusion coefficient of the granules, \( \Theta_i \) is the temperature of the solid phase granules, \( \gamma_{\Theta_i} \) is the energy dissipation due to the particles collision, \( \phi_j \) is the energy exchange between \( i \)-th solid phase and \( j \)-th liquid (gaseous) phase.

The recorded equations system is unclosed. To close the system we use the relationships obtained from the experimental studies of the fluidized bed. The interphases interaction coefficient is determined experimentally and depends on the type of the interacting phases. For two types of phase: liquid (gaseous) phase (\( i \)-th) – solid granular phase (\( j \)-th) model used in [9], in the case of two solid granular phases is the model of [10]. The energy dissipation \( \gamma_{\Theta_i} \) due to the particles collision is written by the model obtained in [11]. Coefficient of the heat exchange intensity is determined for the interaction of two phases by the relation, given in [12]. The motion considered in the reactor at the accepted loads of the raw gas feeding and parameters of the used catalyst is turbulent. In the model accepted for the calculations a dispersion \( \kappa - \varepsilon \) model of turbulence was used in which the motion of "secondary" solid granular phases is generated on the background of the turbulent motion of "primary" gas phase.

2.2. CFD solver
In this paper differential equations that describe the hydrodynamic and thermal processes in the computational model were solved in CFD ANSYS Fluent for unsteady flow regime. The whole computational domain was divided into elements of a triangular or rectangular shape in different subregions, the dimensions of which are sufficient to determine the characteristic factors of the investigated phenomenon. For a given initial distribution of the catalyst in the reactor, after a while the solution reached quasi-stationary regime, at which characteristic hydrodynamic and thermal pictures were calculated.

Boundary conditions were set on all elements of each constructed model of apparatus in accordance with the mechanism of work and the solver used. Since the reactor model assumes rotationally symmetric, then on the axis of the constructed model conditions of axial symmetry «axis» were set. In all non-permeable surfaces «wall» conditions were accepted. In models of raw gas feeder nozzle and in the outlet of the centrally located pipe of the catalyst feed were set «velocity-inlet» (the value of the flow rate) conditions. In the area at the top of the apparatus model there were «outflow» (free flow yield) conditions.
3. Results and discussions
From the analysis of the fractional composition of the catalyst used in the reactor two following models are assumed: monodisperse model with a mean particle size of 80 \( \mu m \) and two-fractional model with a large particle size of 80 \( \mu m \) and with small particles (15% of the total volume of particles) size of 40 \( \mu m \). The gas feeding rate in the calculations corresponds to the average velocity over the apparatus section of 0.3m/s.

3.1. A case with central pipe
Figure 2 shows the characteristic pattern of catalyst particles concentration fields: monodisperse and polydisperse (two fractional). Concentration scale varies from zero to a dense bed catalyst concentration (60% of the volume fraction of the catalyst material considering its voidage). This picture corresponds to the instantaneous state. The monodisperse representation of the fluidized bed particle size is chosen based on that the average velocity of the gas is not enough for the catalyst granules ablation. This ensures that there is the upper boundary of the layer. In turn, the fine particles rise up with the gas flows and circulate throughout the apparatus working area.

![Figure 2. The catalyst concentration field and the temperature filed for the case with a centerline pipe: monodisperse (a), two-fractional (b).](image)

Also, the figure shows the temperature fields. The flow rate of the studied chemical reaction depends on the temperature and occurs with heat absorption. In order to maintain a temperature sufficient for the reaction hot new catalyst is continuously fed into reactor. It is seen, that in the case of monodisperse catalyst the area in the upper part of the apparatus becomes more heated. This is due to the fact that the feed of heated catalyst carried under the base layer and the rising up gas flows take most of the heat from the received catalyst particles. In turn, the heated gas is in a catalyst-free zone, where the flow of chemical reaction is unlikely.

In the presence of small particles the pattern of the temperature field is different. Bottom and middle part of the apparatus occur more heated. This is due to the wall effect along a centerline pipe. Circulating fine particles press the incoming hot catalyst to the pipe, which thin layer flows into the bottom zone of the apparatus, where is a large amount of coarse catalyst. Thus, the presence of fine particles has a positive effect on the heating of apparatus zones and on the chemical reaction rate.

3.2. A case without central pipe
Let us consider the case, when the pipe for the heated catalyst feeding is not vertical, but, for example, is situated from the side. This eliminates the wall effect of the catalyst rolling down. Figure 3
shows the field of catalyst concentration and temperature fields. Almost there is no difference between two concentration patterns from the version with centerline pipe.

However, when considering the temperature fields there are significant differences. The received catalyst gives off heat to the rising gas, as in the case of monodisperse catalyst, or falls into a zone with a sparse fine fraction in the case of two-fractional catalyst. As a result, larger catalyst particles located at the bottom of the apparatus are heated very slowly, which adversely affects the chemical reaction.

4. Conclusion

Thus, indirect structural feature as the location of the pipe to the point of heated catalyst feeding can have a significant impact on the heating of the whole apparatus. Slight movement of the catalyst along pipe (in comparison with the global circulation streams in the apparatus) can have an impact on the processes of heat transfer. In the temperature-dependent processes (chemical reactors) it can be crucial for the apparatus efficiency.

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