Investigation of internal elements impaction on particles circulation in a fluidized bed reactor

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Abstract. A numerical study of the fluidized bed apparatus in the presence of various internal elements is carried out. A chemical reaction for temperature-dependent processes with heat absorption is considered. The task of incoming heated catalyst granules to the reactor is investigated. The main emphasis is focused on the circulation flows of the catalyst particles, heating of the reactor, and the efficiency of the chemical reaction. The analysis of the impact of various design elements on the efficiency of the reactor is carried out. The influence of feeding heated catalyst device design on the effectiveness of whole reactor heating is educed. The influence of the presence of fine particles on the efficiency of the reaction for different reactor design features is also educed.

1. Introduction
Fluidized bed apparatuses are widely used in the chemical industry [1-3]. Their advantage is the high speed of heat and mass transfer between components of the reaction which are resided in different aggregation states. Numerical calculations of fluidization are usually based on Eulerian-Eulerian approach when the carrier (gas, liquid) and the discrete (solid) phase are considered as continuous. To account for the interaction of particles in the fluidized bed, by analogy with the kinetic theory of gases, we added an equation describing the change in the kinetic energy of particles due to their collision (e.g., [4]). Solving these equations numerically allows to carry out calculations of different possible mechanisms of the fluidization process, both in terms of foundational research and practical application.

Each element of the chemical fluidized bed reactor can have a significant impact on hydrodynamics, processes of heat and mass transfer, and the overall efficiency of the apparatus. For example, obviously the shape of the gas feeder will affect the particle motion. Modelling and comparative analysis of two large fluidized bed units with various feed gas supply devices are carried out in [5]. A downward movement of the solid particles along the walls with a high particle concentration is observed in fluidization in cylindrical columns. This effect ensures continuous circulation of the particles in the apparatus. The location of internal elements on the way of the particles main flow stream may affect the operation of the apparatus as a whole. This may improve the chemical reactions efficiency by optimum distribution of the catalyst in the gas flow in the chemical reactors catalytic processes. The changes in the character of the movement and particles concentration along the wall with deflectors are shown in [6]. The works [7, 8] concentrate on the experimental and
numerical study of the ring baffles located on the walls of cylindrical apparatus effect on the hydrodynamics of the fluidized bed.

In this paper we consider the fluidized bed apparatus of cylindrical shape with a uniform gas feeding. The ring baffles, defectors and the grids were investigated as the internal components. The aim of the present paper was to determine the influence of the internal elements on the circulation flow of gas and particles in the apparatus. The pictures of the main circulating catalyst stream were created and the results of the catalyst influence on the concentration were determined. The effect of internal elements on the behavior of the catalyst in reactor and the efficiency of chemical were investigated.

2. Problem formulation and mathematical model
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 $550 \, ^{\circ}C$. There are microspherical catalyst particles with the diameter of 20-200 $\mu m$ in the apparatus. Along the axis is located a vertical pipe for the feeding of the heated catalyst regenerated at $650 \, ^{\circ}C$. In the middle of the reactor, in the working area, are located angular falling through type grids with the free-sectional area approximately of 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. Scheme of considered reactors](image)

The main objective of the article is to determine the hydrodynamic and thermal characteristics of the processes taking place in the reactor for the various constructive scheme of internal elements. We also consider the options without grids, with the ring baffles located on the walls and the other ones.

2.1. Fluidized bed model
Continuous multi-phase Eulerian-Eulerian 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.

Conservation of mass

$$\frac{\partial \alpha_i \rho_i}{\partial t} + \nabla \cdot (\alpha_i \rho_i \vec{v}_i) = 0,$$  (1)

where $\alpha_i$ is the volume fraction of the $i$-th phase, $\rho_i$ is the real density, $\vec{v}_i$ is the velocity.
Conservation of momentum

\[ \frac{\partial \alpha_i \rho_i \vec{v}_i}{\partial t} + \nabla \cdot \left( \alpha_i \rho_i \vec{v}_i \vec{v}_i \right) = -\alpha_i \nabla p + \nabla \cdot \vec{F}_i + \alpha_i \rho_i \bar{g} + \sum_j \vec{R}_y, \]  

where \( \vec{F}_i = \alpha_i \mu_i \left( \nabla \vec{v}_i + \nabla \vec{v}_i^T \right) + \alpha_i \left( \lambda_i - (2/3) \mu_i \right) \nabla \cdot \vec{v}_i \bar{I} \) is the stress tensor, \( p \) is the pressure, \( \mu_i, \lambda_i \) are shear and bulk viscosity, \( \bar{I} \) is a unity tensor, \( \vec{R}_y = K_y \left( \vec{v}_i - \vec{v}_j \right) \) is the force of interphase interaction.

Conservation of energy

\[ \frac{\partial \alpha_i \rho_i h_i}{\partial t} + \nabla \cdot \left( \alpha_i \rho_i \vec{v}_i h_i \vec{v}_i \right) = \alpha_i \frac{\partial p_i}{\partial t} + \vec{F}_i : \vec{v}_i + \sum_j Q_{ij}, \]  

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 [9]:

\[ \frac{3}{2} \left[ \frac{\partial}{\partial t} \left( \alpha_i \rho_i \Theta_i \right) + \nabla \cdot \left( \alpha_i \rho_i \vec{v}_i \Theta_i \right) \right] = \left( -p_i \bar{I} + \nabla \cdot \vec{F}_i \right) \cdot \vec{v}_i + \nabla \cdot \left( k_{\Theta_i} \nabla \Theta_i \right) - \gamma_{\Theta_i} - \phi_{ij}, \]  

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, \( \phi_{ij} \) is the energy exchange between \( i \)-th solid phase and \( j \)-th gaseous phase.

To close the system 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 [4], 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" gaseous 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.
2.3. Chemical reaction efficiency

To estimate the characteristics of the reaction kinetics and apparatus efficiency the simplified chemical reaction efficiency function for control volume was introduced as

$$F_{\gamma}(x, y, z) = V_{cat}(x, y, z)T_{gas}(x, y, z),$$

(5)

where $V_{cat}(x, y, z)$ is catalyst volume of fraction, $T_{gas}(x, y, z)$ is gas temperature at a point of reactor.

The higher gas temperature and the catalyst concentration in the reactor point is more preferable for the chemical reaction at this point. To determine the integral value for total reactor unit volume $V$ characterizing the efficiency function, we consider the coefficient

$$C_{\gamma} = \left( \frac{\int_{V} F_{\gamma} dv}{V_{cat,\max} T_{gas,\max} V} \right) * 100.$$  

(6)

3. Results and discussions

Figure 2 demonstrates the pictures of temperature fields which are shown on a scale from gas feed flow temperature (blue areas) to the temperature of the catalyst feed (yellow areas). The basic case of the reactor in the presence of a central pipe for the heated regenerated catalyst and grids in the cross sections of the block (figure 2, a). Large concentration is observed in the upper part of the apparatus not occupied by the coarse particles. When considering the monodisperse catalyst, the heated particles received through a pipe roll along the pipe wall to the bottom part of the block. The presence of the grids contributes to the appearance of longitudinal fluctuations due to the additional obstacles they create on the way of ascending granules. Thus, the catalyst gives heat off to the incoming gas and the particles in the space between grids and hitting the bottom of the reactor rises up slowly heating the gas and the particles that are in the block. The presence of fine particles changes the picture of the temperature field in the block. The reactor is warmed up slower than in the case of coarse particles only. The fine particles form their own fast circulating flow in the upper part of the block, so that there are large particles too. The heated particles partially roll down along the pipe and are partially entrained by the circulating flow of fine particles. There is a small amount of particles at the top of the block and they quickly transfer the heat to upward feed-gas, which in turn rapidly leaves the reactor. Thus, a substantial portion of the heat is transferred to the gas in the area with a low content of catalyst particles.

![Figure 2](image)

**Figure 2**. Temperature fields for considered cases with monodisperse and polydisperse particles

To evaluate the effect of the grids on the block the heating calculations were also performed in the absence of the grids (case 2, figure 2, b). The reactor temperature was lower compared to a case 1 both for the monodisperse catalyst and in the presence of the fine particles. The reason for it is the coarse particles form a fast circulating flow in the lower part of the apparatus. After getting down the heated
particles rise up faster and give off the heat to the gas at the boundary of large particles. The same happens in the presence of fine particles. Two fast circulating flows of the fine particles in the upper part and the large particles at the bottom of the reactor can be observed.

In the third case (figure 2, c) the location of ring baffles on the walls of the reactor in the absence of grids in the central part of the block is considered. This is done in an attempt to eliminate the fast circulating flow of the case 2 while maintaining a uniform concentration of catalyst. The analysis of the calculation results of case 3 shows that catalyst concentration fields, temperature fields, and circulation flows are in the intermediate state between the cases 1 and 2. Despite the presence of large deflectors, there is upstream large catalyst particles flow around them. The total flow circulation rate slows down, which is beneficial to heat exchange with the gas-feed compared to the case 2. The presence of fine particles has the same effect as in the above cases 1 and 2. However, in this case there is a wide and complex zone of large and small particles circulating streams conjugation due to the presence of deflectors on the walls.

Another option of the construction may consist in a removal of the vertical feed pipe of the regenerated catalyst (figure 2, d). Let’s assume an option (case 4) when the pipe enters the block from the side and in our model is simulated by the insulated feed channel above the top grid. As in case 1, the coarse particles move slowly in the bottom part of the apparatus, and the fine particles form a fast circulating flow in the upper part of the block. However, unlike the case 1, the heated particles get to the upper grids and begin to engage in circulating currents of coarse or fine particles. The pictures of temperature fields show that the lower part of the reactor is hardly warmed. Thus, the particles transfer heat to feed-gas in the middle of the block where the particle concentration is low. Also the calculations without grids (case 5, figure 2, e) but with annular baffles (case 6, figure 2, f) as in the cases 2 and 3 were carried out.

To analyze the efficiency of the chemical reaction we are interested in the previously described coefficients were counted based on catalyst concentration and gas temperature. The results are shown in table 1.

| Case                           | Efficiency 1 fraction of catalyst | Efficiency 2 fractions of catalyst |
|-------------------------------|----------------------------------|-----------------------------------|
| Case 1: central pipe, grids   | 2.622                            | 1.696                             |
| Case 2: central pipe          | 1.695                            | 1.139                             |
| Case 3: central pipe, ring baffles | 1.735                        | 1.376                             |
| Case 4: without central pipe, grids | 0.066                           | 0.097                             |
| Case 5: without central pipe  | 0.032                            | 0.089                             |
| Case 6: without central pipe, ring baffles | 0.017                           | 0.065                             |

It is seen that in the presence of the central vertical pipe the efficiency is much higher. This result is achieved by a fast downflow of the heated particles entering the reactor. This mechanism ensures the feed of regenerated particles into the bottom of the block where they are involved in heat transfer and circulation of the dense bed of large particles. In turn, the presence of small particles for cases 1, 2 and 3 results in the decrease of efficiency since partially regenerated particles are captured by the fast stream and appear at the top of the apparatus. However, for cases 4, 5 and 6 the presence of the fine particles increases the efficiency of the chemical reaction. In the absence of a vertical pipe as the primary mechanism for the initial movement of the regenerated particles (cases 4, 5, 6) heated granules received in the reactor are entrained in the main circulating flows of the apparatus. Since the fine particles move faster along all the reactor height they contribute to the more rapid penetration of incoming particles into the bottom of the block where a dense bed of coarse particles is located. In these cases, the presence of fine particles allows to obtain the greater efficiency in comparison with monodisperse catalyst.
4. Conclusion
Each reactor has its design features which can have a significant effect on hydrodynamics and heat transfer in a fluidized bed. The reactor central pipe has a significant impact on the heating, providing a mechanism for the initial movement of the heated catalyst particles received into the bottom of the unit. The presence of fine particles provides a fast circulating flow in the upper part of the reactor which can have both positive and negative effect on unit performance, depending on the design features of the apparatus. The most effective design features are those that provide a slow movement of coarse particles, a dense bed located in the lower part of the apparatus. Results of this research may be useful in the calculation and design of the fluidized bed apparatus. It should be noted though that each apparatus has its own individual features that can change the representation of the discontinuous phase circulation and heat transfer significantly.

5. References
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