Investigation of the influence of fine particles on the discrete phase density in the numerical modelling of a fluidized bed

S A Solovev¹, ², O V Soloveva³ and A V Antipin⁴

¹Institute of Mathematics and Mechanics, Kazan Federal University, Kremlevskaja st. 18, Kazan, 420008, Russia
²Institute of Mechanics and Engineering – Subdivision of the Federal State Budgetary Institution of Science “Kazan Scientific Center of the Russian Academy of Science”, Lobachevsky st. 2/31, Kazan, 420111, Russia
³Institute of Heat Power Engineering, Kazan State Power Engineering University, Krasnoselskaja st. 51, Kazan, 420066, Russia

E-mail: serguei_s349@mail.ru

Abstract. In this paper, we consider methods for selecting effective diameters of solid particles for simulating a fluidized bed using the Eulerian-Eulerian approach in order to describe a multiphase medium. Calculations for modal mean diameter and mean diameter of Sauter were carried out. Studies have also been carried out for the bidisperse composition of the particles, with separation into coarse and fine fractions. The results of the numerical simulation were compared with the data from experimental studies.

1. Introduction
The high intensity of heat and mass transfer processes in a fluidized bed apparatus allows to effectively conduct catalytic chemical reactions [1, 2]. The catalyst is a mixture of approximately spherical solid particles of different diameters, forming a discrete polydisperse phase. The polydisperse properties of the particle mixture are taken into account by the probability distribution function (PDF) of the particle diameters.

In the numerical modelling of a fluidized bed, the Euler-Euler model of a multiphase medium in which the phases are considered as interacting and interpenetrating continuum is widely used. This approach requires the discretization of the particle characteristics. Discretization can be carried out using a multi-group approach, the essence of which is to divide the domain of definition of PDF into groups of diameters and to assign them a certain value of the cumulative distribution function (CDF), which characterizes the fraction of the group in the bed of particles, with the transfer equations being solved for each group separately. The multi-group approach was used for numerical modelling of gas–solids flow in [3, 4]. In work [5] shown that the method of polydispersity accounting can influence the hydrodynamic characteristics of the flow obtained in the calculation. It was shown in [5] that the method of taking into account the polydispersity can affect the hydrodynamic characteristics of the flow obtained in numerical simulation.

Thus, a universal method of discretizing the characteristics of polydisperse solid particles is needed. The method should provide the optimal choice of the smallest number of particle fractions for numerical calculation and reflect the effects associated with polydispersity.
2. Problem formulation and experimental study

2.1. Experimental setup
The scheme of the experimental setup, which is a high glass tube with an internal diameter of 2.2 cm, is shown in Fig. 1. The porous material is located at the bottom of the tube, which ensures a uniform flow of air supplies from the compressor. The volume flow rate was measured at the output of the tube using a rotameter. Fluidization process was filmed on high-speed camera, the height of a bed was estimated by shots from the camera.

![Diagram of experimental setup](image)

*Figure 1. Scheme of experimental setup.*

2.2. Material properties
Polydisperse system of a microspherical chromia-alumina catalyst particles with diameters 20 - 140 micrometers designed for dehydrogenation of isobutane, belonging to the Geldart group B, were investigated. The cumulative particle size distribution (CDF) is given in Table 1. CDF, PDF, and discrete particle size probabilities shown on Fig. 2. Air was used as a fluidizing agent.
The advantage of the Euler-Euler approach of numerical fluidization modelling is relatively small computational costs. Such an approach to modelling a fluidized bed requires the discretization of the characteristics of the particles. In this paper, we consider methods of discretization based on effective diameters (1) and the terminal velocity (2) of the particle. The essence of the method is to obtain two effective diameters, the first for large heavy particles forming a dense phase, and the second for small particles carried away by the flow.

$$D_{32} = \frac{\int_{D_{32}}^{\infty} f(D)D^2dD}{\int_{0}^{\infty} f(D)D^2dD}, \quad D_{\text{mod}} = \arg\max_D \left( f(D) \right). \quad (1)$$

Figure 2. Particle characteristics.

Table 1. Cumulative distribution of particle size

| Particle size (µm) | % in a bed |
|-------------------|------------|
| 22.909            | 0          |
| 26.303            | 0.2        |
| 30.20             | 0.3        |
| 34.674            | 2.26       |
| 39.811            | 8.17       |
| 45.709            | 20.28      |
| 52.481            | 38.55      |
| 60.256            | 59.62      |
| 69.183            | 78.38      |
| 79.433            | 91.16      |
| 91.201            | 97.54      |
| 104.713           | 99.72      |
| 120.226           | 100        |
| 138.038           | 100        |
First, equating the known gas velocity \( u_g \) to the terminal velocity (1), it is necessary to obtain a diameter \( D_s \), with respect to which the initial mixture of particles can be divided into two groups described above. \( D_s \) is a root of the equation (3).

\[
\begin{align*}
\frac{\rho_f}{\mu_f} &\leq 0.4, \quad \text{Re}_p = \frac{\rho_f |u_p - u_s| D}{\mu_f} < 200000. \\
\end{align*}
\]  

Initial volume fraction for both diameters can be obtained by a fixed bed volume fraction of particles mixture \( \alpha_0 \) and CDF of particles diameters.

\[
\alpha_1^i = \alpha_0 \text{CDF}(D), \quad \alpha_2^i = \alpha_0 (1 - \text{CDF}(D)).
\]  

Effective diameters and volume fractions for conducting experiments calculated by the algorithm described above are presented in Table 2.

| Fluid velocity (m/s) | Fine particle diameter (µm) | Coarse particle diameter (µm) | Fine particle volume fraction | Coarse particle volume fraction |
|----------------------|-----------------------------|-------------------------------|-------------------------------|-------------------------------|
|                      | \( D_1 \)                   | \( D_2 \)                     | \( D_1 \)                     | \( D_2 \)                     | \( \alpha_0 \)                 | \( \alpha_0 \)                 |
| 0.0716               | 30.5                        | 32.4                          | 66.9                          | 56.4                          | 0.005                          | 0.411                          |
| 0.0892               | 33.4                        | 35.6                          | 67.2                          | 56.4                          | 0.014                          | 0.402                          |
| 0.1088               | 36.4                        | 39.6                          | 67.7                          | 56.4                          | 0.033                          | 0.383                          |
| 0.1213               | 38.2                        | 42.0                          | 68.3                          | 56.4                          | 0.052                          | 0.364                          |

2.3. Experimental data
The experiments were carried out for gas velocities at which small particles were carried away. There were significant fluctuations in the height of the bed. All tests were conducted for 30 grams of
catalyst, the initial volume fraction of solid particles in the fixed bed was $\alpha_0 = 0.41639$. The results of measurements of heights are given in Table 3.

| Fluid velocity (m/s) | Observed minimum height (m) | Mean height (m) | Observed maximum height (m) |
|----------------------|-----------------------------|----------------|---------------------------|
| 0.0716               | 0.107                       | 0.1386         | 0.19                      |
| 0.0892               | 0.12                        | 0.1433         | 0.18                      |
| 0.1088               | 0.13                        | 0.1683         | 0.23                      |
| 0.1213               | 0.13                        | 0.1721         | 0.24                      |

### 3. Numerical study

#### 3.1. Fluidized bed numerical model

The numerical simulation of a fluidized bed was performed via continuous multiphase Eulerian-Eulerian model coupled with the kinetic theory to include the interaction between solid particles. In the present study the following equations were solved:

**Conservation of mass**

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

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**

$$\frac{\partial \alpha_i \rho_i \vec{v}_i}{\partial t} + \nabla \cdot (\alpha_i \rho_i \vec{v}_i \vec{v}_i) = -\alpha_i \nabla \rho + \nabla \cdot (\vec{p} + \alpha_i \rho_i \vec{g}) + \sum_j R_{ij},$$

where $\vec{p} = \alpha_i \mu_i \left( \nabla \vec{v}_i + \nabla \vec{v}_i \right) + \alpha_i \left( \lambda_i - (2/3)\mu_i \right) \nabla \cdot \vec{v}_i \vec{T}$ is the stress tensor, $\rho$ is the pressure, $\mu_i, \lambda_i$ are shear and bulk viscosity, $\vec{T}$ a unity tensor, $R_{ij} = K_{ij} \left( \vec{v}_i - \vec{v}_j \right)$ is the force of interphase interaction.

The equation for granular temperature takes the form [6]

$$\frac{3}{2} \frac{\partial}{\partial t} \left( \alpha_i \rho_i \Theta_i \right) + \nabla \cdot \left( \alpha_i \rho_i \vec{v}_i \Theta_i \right) = -p_i \vec{v}_i + \vec{p}_i \nabla \vec{v}_i + \nabla \cdot \left( k_{\Theta_i} \nabla \Theta_i \right) - \gamma_{\Theta_i} + \phi_{\Theta_i},$$

where $k_{\Theta_i}$ is the diffusion of energy coefficient, $\Theta_i$ is granular temperature, $\gamma_{\Theta_i}$ is collisional dissipation of energy, $\phi_{\Theta_i}$ is the energy exchange between the gas phase and the solid phase.

The system of equations was closed by semiepirical models of interphase interaction. For liquid (gaseous) phase ($i$-th) – solid granular phase ($j$-th) interaction were used from [7], in the case of two solid granular phases is the model of [8]. The energy dissipation $\gamma_{\Theta_i}$ due to the particles collision is written by the model obtained in [9].

#### 4. Results

The results of numerical simulation using the methods for selecting effective diameters were compared with the experimental data, as well as with the results of calculations carried out with one effective diameter. The distribution of the catalyst volume fraction of tube height, obtained in the calculations, is shown in Fig. 3.
Figure 3. The distribution of the particle volume fraction along the height of the tube for four values of the flow velocity.

It is seen that in all calculations the height of a dense particle bed is within the limits of observed minimum and maximum. From Fig. 3 (a) and (b) it can be seen that at low velocities, the addition of fine fraction practically does not affect the average heights of the dense bed obtained in the calculations. This is explained by the fact that the particle volume fraction with a diameter smaller than \( D_f \) is negligible.

Time-averaged bed heights obtained experimentally and numerically, are shown in Fig.4.
The average heights of the dense bed, obtained in the calculations with two effective diameters $D_{32}$ and $D_{32}^2$ for the fine and coarse fractions respectively, showed a better fit to the experiment than the heights obtained from calculations with one effective diameter $D_{32}$. This is indicated by the fact that the standard deviation of the calculated heights from the experimental ones, given in Table 3, for calculation with two fractions less than one fraction. In the case where the effective diameters were chosen as a mode, it turned out that the heights obtained in the calculations with two effective diameters $D_{mod}^1$ and $D_{mod}^2$ turned out to be larger than the experimental mean, moreover, the heights in calculations with one effective diameter $D_{mod}$ turned out to be closer to the experimental mean by the standard deviation.

| Effective diameter | Root-mean-square deviation (m) |
|--------------------|--------------------------------|
| $D_{32}$           | 0.0233                         |
| $D_{mod}$          | 0.0134                         |
| $D_{32}$ coarse    | 0.0190                         |
| $D_{mod}$ coarse   | 0.0294                         |

5. Conclusion

When simulating a fluidized bed using the Euler-Euler approach, the average Sauter diameter $D_{32}$ is taken as the effective diameter of the particle mixture. The use of two effective diameters $D_{32}^1$ and $D_{32}^2$ improves the correspondence of calculations to experiment on the parameter of the average particle density in the layer. In this case, the opposite situation occurs with modal effective diameters $D_{mod}^1$ and $D_{mod}^2$. The average heights obtained in calculations with one effective diameter $D_{mod}$ showed the smallest standard deviation from the experimental mean altitudes, but with increasing gas velocity, such a phenomenon as the removal of fine particles becomes more pronounced. This fact cannot be reflected in calculations with one effective diameter.
In this paper, it was established that for the particle mixture considered, the experimental mean height is greater than the dense-bed height obtained in calculations with two effective diameters $D_{32}^1$ and $D_{32}^2$, and do not exceed the heights of the dense-bed obtained in the calculations for $D_{mod}^1$ and $D_{mod}^2$. On the basis of this fact, for a particle mixture with a similar distribution function, the following conditions for choosing effective diameters can be recommended

$$D_{32}^1 \leq D_{ef}^1 \leq D_{mod}^1, \quad D_{32}^2 \leq D_{ef}^2 \leq D_{mod}^2.$$  

(9)

Acknowledgments
The reported research was funded by Russian Foundation for Basic Research and the government of the Republic of Tatarstan of the Russian Federation, grant № 18-48-160006.

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