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System approach to calculating processes in the apparatus of combined action

Abstract

A method of calculating the apparatus of combined action for carrying out a high-temperature reaction in a fluidised bed of the solid reactant particles is proposed based on a system approach. In this bed, the reaction proceeds simultaneously with the continuous grinding of the formed products and the processes of heat and mass transfer are significantly intensified in connection with the constant renewal (denudation) of the reaction surface both due to the impact fracture of the product shell in the zones of the intensive collision in the counterflows of the reacting particles and its abrasion in the body of the fluidised bed.

Keywords: apparatuses of combined action, fluidised bed, system approach

Streszczenie

W pracy zaproponowano algorytm obliczeń młyna strumieniowego, w którym przebiega wysokotemperaturowa reakcja w złożu fluidalnym cząstek stałych – reakcja przebiega równocześnie z mieleniem cząstek w złożu. Transport ciepła i masy są znacznie zintensyfikowane w związku z ciągłym odnawianiem (denudacją) powierzchni reakcji zarówno ze względu na pęknięcia udarowe powłok reagujących cząstek, jak i ich ścieranie w złożu fluidalnym.

Słowa kluczowe: młyn strumieniowy, złoże fluidalne, algorytm obliczeń

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1. Introduction

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An apparatus of combined action or an apparatus with several sequential or serial/ parallel processes combined in one casing may be classified as a rather complicated chemical – engineering system in order of complexity of interaction.

A high-temperature reactor in the gas-solid system, in which the reaction products formed on the solid reactant particles significantly slow down the processes of heat and mass transfer to the boundary of the reaction, may serve as an example of a system approach to the calculation of the combined processes $\lceil 1-3 \rceil$.

One of the problems of calculating these apparatuses is to elaborate a mathematical model of the hydrodynamics of a two-phase high-speed jet that develops in a fluidised bed with the determination of the concentration of solid particles in the jet and velocity of their motion, followed by the subsequent computation of the probability of collision and destruction of particles in the opposite jets and estimation of the particle size distribution after the collision.

2. Hierarchy structure for calculating the apparatus of combined action

The processes occurring in the apparatus of combined action are divided into the following main levels (subsystems) as a complex hierarchy system: the process of grinding of the reacting particles in a fluidised bed with built-in zones of intense destruction of the formed reaction products due to the acceleration and collision of particles in the countermoving jets and heat and mass transfer processes.

In turn, the level (subsystem) of grinding is subdivided into its subordinate levels as follows:

- a) the determination of the motion velocities of the particles in the zones of their impact collision;
- b) the calculation of the process of grinding at their collision in counterflow jets.

It is reasonable that the heat and mass transfer processes are investigated starting with the processes that take place in a single particle.

In the general case, the structure for calculating the combined apparatus of this type can be represented by the following flowchart shown in Fig. 1.

In the present paper, due to the large amount of the data, only the subsystem concerning the process of grinding of the reaction products is discussed.

To intensify the process of a chemical reaction in a solid particle, the grinding should occur at rates close to the rate of a chemical reaction in order to exclude the possibility of the diffusion resistance in the shell of the forming product. At the same time, the particles obtained from grinding should exhibit a predetermined degree of dispersion, high chemical activity, and a high degree of conversion.

The apparatus that combines grinding of the material and the reaction products under a high impact loading in a fluidised bed of the particles, in which an endothermic chemical reaction is carried out either due to the heat of the gas supplied to the fluidisation or the burning of gas in a bed under the implementation of high temperature processes, satisfies these requirements. The classification of particles by size is also performed inside of the apparatus using the inertialpneumatic classifier. The main grinding is carried out by an acceleration of particles by a gas jet and their collision in counterflow jets directly inside the fluidised bed. The majority of fine particles are generated due to the abrasion of fragments formed within the fluidised bed. The apparatus operates without barring tubes and remote overflow devices since their application at high ambient temperatures and increased abrasiveness of the material being worked is very difficult. For the same reasons, the use of an apparatus of complex design as a classifier is also unacceptable.

Fig. 1. Flowchart of calculating apparatus of combined action

The three main problems of calculating such apparatus are as follows: the determination of the average time of the location of decarbonized and decomposed particles inside the apparatus, the evaluation of its productive capacity and the particle size distribution of the fine product, as well as the calculation of the apparatus dimensions using the pre-assigned capacity.

The complexity of the computation lies in the fact that all technological processes that take place in the apparatus under discussion are interrelated as well as interdependent and occur simultaneously. The transient operating mode of the apparatus is observed at a period from its starting up to the moment when a balance between the entry of the material into the apparatus and the mass flow rate of the final product is established.

The description of the hydrodynamic conditions in the apparatus is confined to a modelling of the processes in different zones, which can be distinguished within the apparatus. The main zones or subsystems of the process of the destruction of the reaction products are highpressure two-phase jet, a core of collision of counterflow jets, fluidised bed, a separation zone.

Knowledge of the particle size distribution of the granular material in each subsystem is required to describe the hydrodynamics of any of the selected subsystems. Certain difficulties emerge when a particle size distribution is calculated at each section since in the operating process of the apparatus, a constant exchange of the material particles between the selected zones takes place. Before the establishment of the transient operating mode of the apparatus, i.e., until the moment when a fluidised bed of a constant volume and particle size distribution is accumulated, the particles not only from the surrounding bed, but also immediately from the feed nozzle enter a high-pressure jet of the energy carrier. Thus, the particulate matter with a varying particle size distribution enters the zone of collision of the counterflow jets, i.e. the core of collision.

Fig. 2. Schematic diagram of the apparatus of combined action: 1 – outlet nozzle; 2 – reaction chamber; 3 – delivery nozzles; 4 – combustion chamber; 5 – gas distribution grid; 6 – inertialpneumatic classifier

Fig. 3. Schematic structure of the dispersed phase flows in the apparatus of combined action

The solution of the problem of calculating the particle size distribution at each zone (subsystem) of the combined apparatus is possible if the time until the establishment of the stationary mode is divided into n time intervals and the calculation is carried out by stages with regard to the structure of solid streams between the characteristic subsystems of the apparatus. This structure is shown in Fig. 3.

The calculation is performed as follows:

1) $\tau = t_1$

$$
J_1^{grind} \cdot F_1^{grind} (d) = J^{in} \cdot F_{init} (d) \rightarrow J_1^{grind} \cdot F_{1k}^{grind} (d)
$$
\n
$$
J_1^{d} \cdot F_1^{d} (d) = \frac{\sum_{d_{bound}}^{d_{max}} J_1^{grind} \cdot F_{1k}^{grind} (d) \cdot \eta (d)}{\sum_{d_{min}}^{d_{max}} J_1^{grind} \cdot F_{1k}^{grind} (d)}
$$
\n
$$
J_1^{out} \cdot F_1^{out} (d) = \frac{\sum_{d_{bound}}^{d_{bound}} J_1^{grind} \cdot F_{1k}^{grind} (d) \cdot \eta (d)}{\sum_{d_{min}}^{d_{max}} J_1^{grind} \cdot F_{1k}^{grind} (d) \cdot \eta (d)}
$$
\n
$$
J_1^{bed} \cdot F_1^{bed} (d) = (1-k) \cdot J_1^{d} \cdot F_1^{d} (d)
$$

2) $τ = t_2$

$$
J_2^{grind} \cdot F_2^{grind} (d) = J^{in} \cdot F_{init}^{in} (d) + k \cdot J_1^{cl} \cdot F_1^{cl} (d) \rightarrow J_2^{grind} \cdot F_{2k}^{grind} (d)
$$

$$
J_2^{cl} \cdot F_2^{cl} (d) = \frac{\sum_{d_{bound}}^{d_{max}} J_2^{grind} \cdot F_2^{grind} (d) \cdot \eta(d)}{\sum_{d_{min}}^{d_{max}} J_2^{grind} \cdot F_{2k}^{grind} (d)}
$$

$$
J_2^{out} \cdot F_2^{out} (d) = \frac{\sum_{d_{bound}}^{d_{bound}} J_2^{grind} \cdot F_{2k}^{grind} (d)}{\sum_{d_{min}}^{d_{max}} J_2^{grind} \cdot F_{2k}^{grind} (d)}
$$

$$
J_2^{out} \cdot F_2^{out} (d) = (1 - k) \cdot J_2^{cl} \cdot F_2^{cl} (d)
$$

n) $\tau = t_n$

$$
J_n^{grind} \cdot F_n^{grind}(d) = J^m \cdot F_{init}^m(d) + k \cdot J_{n-1}^d \cdot F_{n-1}^d(d) \rightarrow J_n^{grind} \cdot F_{nk}^{grind}(d)
$$
 (1)

$$
J_n^{cl} \cdot F_n^{cl}(d) = \frac{\sum_{d_{bound}}^{d_{max}} J_n^{grind} \cdot F_n^{grind}(d) \cdot \eta(d)}{\sum_{d_{min}}^{d_{max}} J_n^{grind} \cdot F_n^{grind}(d)}
$$
(2)

$$
J_n^{out} \cdot F_n^{out}(d) = \frac{\sum_{d_{\min}}^{d_{\text{bound}}} J_n^{grind} \cdot F_{nk}^{grind}(d)}{\sum_{i}^{d_{\text{max}}} J_n^{grind} \cdot F_{nk}^{grind}(d)}
$$
(3)

$$
J_n^{bed} \cdot F_n^{bed}(d) = (1-k) \cdot J_n^d \cdot F_n^d(d)
$$
\n
$$
\tag{4}
$$

where *J^{grind, in c1, out, bed* is the mass flow rate of the solid material after grinding in the jets,} at the inlet to the jet, in the classification zone, at the output from the apparatus, and in a fluidised bed, respectively, kg/s; *F*(*d*) is the column matrix of the particle-size distribution of the material, where the indices are the same as those described above; *d* is a diameter of the solid phase particles, m; t is current time; $\eta(d)$ is the efficiency of the classification process; τ is a time, s; *k* is the proportion of particles which are recycled to the jet for regrinding.

The calculation step is given based on the productive capacity of the apparatus and the time required to achieve the stationary operating mode, i.e.

$$
J^{in}=J^{out}
$$

The calculation is performed until the moment when the most constant particle size composition is fixed that makes it possible to determine the time before the establishment of the stationary mode.

This time is necessary to estimate the mass of the bed of granular material, and therefore, the apparatus dimensions and the pulse rate of compressed air supply at pulse operating mode.

3. Description of hydrodynamics in the high-pressure jet

When analysing the existing methods for calculating the hydrodynamic conditions in the two-phase flow apparatuses (the apparatuses with fluidised, spouted beds, jet grinders, pneumatic conveying systems, etc.), the following most characteristic stages can be distinguished:

- \triangleright the determination of the velocities of gas phase in the jet of the energy carrier in the bed;
- \triangleright the estimation of the solid phase transition velocities in the bed and in the flow;
- \triangleright the calculation of the amount of both phases, which are entrained from the surrounding bed by the energy carrier flow;
- \blacktriangleright the determination of the density of two-phase flow;
- \blacktriangleright the mixing of the solid phase particles within the bed and in the carrier flow;
- \triangleright the evaluation of motion speeds of polydisperse particles in the two-phase jet;
- \blacktriangleright the determination of the concentration of solid phase particles in any arbitrary section of the two-phase jet;
- \triangleright the evaluation of the probability of collision of particles in opposite jets;
- \blacktriangleright the determination of the probability of particles grinding following their collision;
- \triangleright the calculation of the particle size distribution after a single grinding;
- \triangleright the calculation of the process of the abrasion of particles in the bed;
- \triangleright the determination of the number of particles entering the high-speed two-phase jets for the second grinding cycle.

To describe the hydrodynamics of the two-phase jet consisting of a gas and solid material particles, the drift model was used, i.e. the motion of the continuous and dispersed phases was considered independently of one another. To determine the amount of gas entrained from the surrounding fluidised bed by the jet $(j_{\scriptscriptstyle en}]$, the analogy between the free flowing highpressure jet and the jet compressor was applied $[1]$.

The horizontal (axial) velocity component of the entrained gas can be represented as follows:

$$
U_{en} = \frac{J_{en}}{F_{con} \cdot \varepsilon_0 \cdot \gamma_G}; \quad \text{where} \quad J_{en} = J^P \cdot \frac{\varphi}{1 - \varphi}
$$
 (5)

$$
\varphi = 1 - \frac{1}{0.75 + 0.25 \cdot \left(\frac{b_{\text{init}}}{r^{n\alpha}}\right)^2}
$$
(6)

The mixed flow velocity is determined from the following expression:

$$
U_{\text{noz}} = U_{\text{init}} \cdot \left[1 - \varphi \cdot \left(1 - \frac{U_{\text{en}}}{U_{\text{init}}} \right) \right] \tag{7}
$$

Next, the parameters of the gas jet were calculated using a known method proposed by Yu. A. Buevich and G. A. Minaev $(4, 5)$.

The particle motion in the two-phase flow is largely determined by the hydrodynamic force, which depends on the relative velocity of motion of the phases and the hydrodynamic drag coefficient.

It seems that the description of the motion pattern of a solid particle under the influence of the hydrodynamic drag force with regard to the effect on the nature of the motion of

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the constraint of the flow, the presence of other particles in the jet, as well as particle shape coefficient is the most simple and yet sufficiently complete.

The value of the relative velocity of a solid particle at any point of the jet can be determined by the following formula:

$$
V_{i} = \frac{c}{1 - \exp(\tau_{i} \cdot a \cdot c) - \left(\frac{c}{V_{init}}\right) \cdot \exp(\tau_{i} \cdot a \cdot c)}
$$
\n
$$
a = \frac{0.366 \cdot k_{1} \cdot k_{2} \cdot k_{3}}{d} \cdot \frac{\rho_{G}}{\rho_{S} - \rho_{G}}; \quad c = \frac{65 \cdot v}{k_{3} \cdot d}; \quad k_{1} = \varepsilon^{4.75};
$$
\n
$$
k_{2} = \frac{1}{\left[1 - \left(\frac{d}{2 \cdot b_{i}}\right)^{2}\right]^{3}}; \quad k_{3} = 11 - \frac{10}{f}; \quad f - \text{coefficient of particle shape.}
$$
\n(8)

Since the relative velocity of the solid phase particles at the initial stage of the development of the two-phase jet is equal to VXin = Uin - WXin, it is essential to know the initial velocity of the solid material particles WXin accelerated by the gas jet to perform calculations using this formula.

The studies carried out by us demonstrate that the particles have an initial velocity, which is different from zero when they enter a high-speed gas jet from the surrounding fluidised bed, as shown below:

$$
W_{Xin} = \frac{J_S}{F_{con} \cdot \gamma_{bed}} \cdot \sin \alpha \tag{9}
$$

where α is the expansion angle of a gas jet.

Fig. 4. Hydrodynamic characteristics of the two-phase jet: solid lines show absolute axial velocity of the solid phase, dotted lines show axial velocity of the gas phase; $1 - d_p = 2$ mm; $2 - d_p = 3$ mm; $3 - 2$ $d_p = 5$ mm

The calculation of the motion velocity of the solid material particles is performed until the moment of their collision with the particle of the counter flow.

Axial and radial flow velocity components of the solid phase, as well as the particle velocity at the plume boundary, are calculated using the following formulas:

$$
W_{xi} = U_{xi} - V_{xi}; \quad W_{yi} = U_{yi} - V_{yi}; \quad W_b = U_b \tag{10}
$$

The boundary of the collision of counter flows was determined on condition that the particles have attained the velocity, which is optimal for grinding. When considering the motion of a particle beyond the boundary of the collision, it is believed that it is only subjected to the suppressive action of the counter gas flow.

From the calculation data, based on the proposed method, the dependences of the hydrodynamic characteristics of two-phase flow on the particle sizes of the solid phase and the accelerating nozzle were plotted (Fig. 4), as well as the time required for the acceleration of particles to maximum motion velocities and the optimal distance between two opposite high-pressure nozzles were determined.

4. Calculation of the particle size distribution in the core-of-collision

The information concerning the determination of the concentration of the solid-phase particles in any arbitrary section of the two-phase jet, as well as the probability of collision of particles and the probability of their grinding upon the collision of the jets and the calculation of the particle size distribution after a single loading is studied in detail in [2].

Thus, the concentration of particles at the cross-sectional area of the jet $C_{\scriptscriptstyle{F}}$ is determined by the formula

$$
C_F = \frac{1.5 \cdot J_s}{W_{av} \cdot F_s^{phase} \cdot \rho_s}
$$
 (11)

The probability of collision of the solid material particles with each other Pci in the event of their uniform distribution over the cross section of the flow is equal to the arithmetic sum of the cross-sectional areas occupied by the particles in the jet, i.e.

$$
P_{\rm cr} = \sum C_{\rm F} \tag{12}
$$

or, in terms of the movement of the jets to the left and right side from the boundary of the collision,

$$
P_{Cj} = C_{Fj}^{left} + C_{Fj}^{right} \tag{13}
$$

Where *j* is a number of the section of the jet on the longitudinal coordinate.

The zone of collision of particles in the counter flow can be limited and the so-called core of collision or grinding can only be considered. The calculations on the proposed model show that the total probability of collision of particles in the selected core comes close to 70%.

To determine the particle size distribution directly in the core of collision after grinding, the matrix model of grinding described in detail in $[6]$ is used as follows:

$$
F_{\text{fin}}^{\text{grind}}(d) = (1 - P(d)) \cdot F_{\text{init}}^{\text{grind}}(d) + P_p(d) \cdot F_{\text{init}}^{\text{grind}}(d) \cdot \phi(d)
$$
(14)

where the probability of destruction is

t

$$
P_{d}(d) = 2 \cdot P_{av}(d) \cdot \sum_{i=1, j=1}^{j=n} P_{Cij}
$$
 (15)

The probability of grinding of the solid material particles when they collide is determined by the known formula

$$
P = \frac{1}{(2 \cdot \pi)^{0.5}} \cdot \int_{-\infty}^{t} e^{-t/2} dt
$$

= 2.5 · $\lg \frac{W}{W_{cr}}$; $W_{cr} = 1.9 \cdot \frac{\left(\left(\frac{[\sigma]}{\rho_s}\right) \cdot 10^{-3} + 1\right)}{d_{av}^{0.48}}$ (16)

The proposed method for calculating the probability of collision and destruction of the solid material particles in the high-speed counterflow jets of the energy carrier makes it possible to define the productive capacity of the apparatus on the finely dispersed product.

The calculation results for the subsystem under discussion can be seen on the graph representing the changes in the initial particle size distribution of the particulate material at a single grinding in the counter-flow jets (Fig. 5).

Fig. 5. Change in the particle size distribution of the particulate material at a single loading in the grinding core at *rnoz* = 6 mm: 1 – initial particle size distribution; 2 – final particle size distribution

5. Conclusions

In the present paper, a method of calculating the apparatus of combined action that combines the process of a chemical reaction and grinding of the obtained products is investigated. The hierarchical structure for calculating the process of grinding of the reacting particles in a fluidised bed with built-in zones of the intense destruction of the formed reaction products due to the acceleration and collision of particles in the countermoving jets was proposed. The subsystem of the calculation of hydrodynamics of the two-phase high-speed jets and the subsystem of the process of grinding of particles at their collision in counterflow two-phase jets were discussed in detail.

Notation

- *a* tensile strength, MPa;
- *b* radius of the jet plume, m;
- *C* concentration;
- *d* diameter, m;
- *F* surface area, m2;

F(d) – column matrix of the particle size distribution of the material;

- $J -$ mass flow rate, kg/s ;
- *P* probability of grinding;
- *Pc* probability of collision;
- *Pd* probability of destruction;
- *P(d)* diagonal matrix of the probabilities of destruction;
- *r* radius, m;
- U gas phase velocity, m/s;
- *V* relative velocity of the solid phase, m/s ;
- $W -$ absolute velocity of the solid phase, m/s;
- γ specific gravity;
- ϵ porosity;
- η efficiency of the jet;
- v kinematic viscosity of the gas, m2/s;
- σ density, kg/m3;
- τ time, s

Subscripts and superscripts

- *b* boundary of the jet plume;
- *F* surface area;
- *i* calculation step;
- *j* number of the section of the jet on the

longitudinal coordinate;

- *max* maximum value;
- *min* minimum value;
- *n* consecutive number;
- *in* input flow;
- *out* output flow;
- $G gas phase;$
- *bound* boundary value;
- *grind* grinded flow;
- *fin* final value;
- *cl* flow after classification;
- *con* cone;
- *cr* critical value;
- *left* left part;
- *init* initial value;
- *hole* holes of the gas distribution grid;
- *en* entrained flow;
- *right* right part;
- *compr* compression;
- *bed* bed (fluidised);
- *noz* nozzle;
- *av* average value;
- *S* solid phase.

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