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Computational and Experimental Study of the Patterns of Formation of a Fluidized Bed of Inert Haydite Particles Material

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Abstract. At present, an actual trend in the development of fuel and energy complexes in a number of countries is the diversification of generation via the involvement of local types of solid fuel. In this case, thermochemical processing of fuel is often carried out in a fluidized state. A significant proportion of dispersed fuels cannot be transferred to a state of stable fluidization. The solution in such cases is to create a fluidized bed of inert carrier, into which particles of the target fuel component are then introduced. In this work, a computational and experimental study of the fluidization of inert bulk material (haydite granules) was carried out. The key purpose of the work was to develop a mathematical model for the formation of a fluidized bed, which makes it possible to calculate the process based on its local characteristics, as well as to identify the model parameters and test it using experiment data. During the study the problems of developing a numerical method for calculating the distribution of velocities and concentrations along the height of the apparatus were solved, parametric identification of the proposed mathematical model was carried out, and empirical verification of the modeling results was carried out. The mathematical apparatus of the theory of Markov chains was used as the mathematical basis for constructing the model. The data from our own laboratory full-scale experiment were used to identify the parameters of the model and verify it. A comparison of calculated and experimental data showed the high predictive efficiency of the model for the given granulometric composition of the fluidizing product. The results of the laboratory full-scale experiments also showed a significant evolution of the granulometric composition of haydite granules during their long-term stay in a fluidized bed, which requires a separate study, as well as the introduction of appropriate amendments to the mathematical model for its further improvement.

Keywords: fluidized bed, numerical simulation, Markov chains, gas velocity profile, haydite particles

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Расчетно-экспериментальное исследование закономерностей формирования кипящего слоя инертного керамзитового материала

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Реферат. В настоящее время актуальной тенденцией развития топливно-энергетических комплексов ряда стран является диверсификация генерации за счет вовлечения местных видов твердого топлива. При этом термохимическая переработка топлива часто реализуется в псевдоожиженном состоянии. Существенная доля дисперсных видов топлива не может быть переведена в состояние стабильного псевдоожижения. Выходом в таких случаях является создание псевдоожиженного слоя инертного носителя, в который затем вводят частицы целевого топливного компонента. В настоящей работе предпринято расчетно-экспериментальное исследование псевдоожижения инертного сыпучего материала (гранул керамзита). Целью настоящей работы является разработка математической модели формирования псевдоожиженного слоя, позволяющей вести расчет процесса по его локальным характеристикам, а также идентификация параметров модели и ее проверка по данным натурного эксперимента. В ходе исследования решены задачи разработки численного метода расчета распределения скоростей и концентраций по высоте аппарата, выполнена параметрическая идентификация предложенной математической модели, эмпирическая проверка результатов моделирования. В качестве математической основы построения модели использован математический аппарат теории цепей Маркова. Для идентификации параметров модели и ее верификации использованы данные собственного натурного эксперимента. Сравнение расчетных и экспериментальных данных показало высокую прогностическую эффективность модели для известного гранулометрического состава ожижаемого продукта. Результаты натурных экспериментов показали также значительную эволюцию гранулометрического состава частиц керамзита при их длительном пребывании в псевдоожиженном слое, что требует отдельного исследования, а также введения соответствующих поправок в математическую модель для ее дальнейшего совершенствования.

Ключевые слова: псевдоожиженный слой, численное моделирование, цепи Маркова, профиль скорости газа, частицы керамзита

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Introduction

Currently, the efforts of many countries are aimed at improving technologies for processing solid fuels and increasing electricity generation through the use of various types of renewable solid fuels [1–3]. These trends are supported by very reasonable considerations. The use of renewable local solid fuels allows for diversification of generation and provides affordable, functional and sustainable energy in all weather conditions for rural electrification [4]. Compared with fossil fuels, the use of biomass also supports the trend towards transition to more clean and low-carbon energy systems [4, 5]. Due to the desire to intensify 334

technological processing processes, industry traditionally uses equipment with active hydrodynamic flow regimes [6–8]. These apparatuses can be divided into three groups depending on the flow configuration of the combustor: vortexing, swirling and cyclonic fluidized-bed combustors [9–11]. However, some granular media due to its physical and mechanical characteristics do not form a sufficiently stable and predictable fluidization pattern [12–15]. Researchers associate the reasons for these difficulties with the peculiar shape of the particles, which is characterized by many objective characteristics (particles sizes, densities, shapes, proportions etc.) [13–15]. The peculiar shape of fluidization, elutriation, and segregation [14, 15]. These difficulties are noted by many researchers when fluidizing many types of local bulk biofuels: rice husk [16, 17], cotton stalk [13], palm shell [18] etc. To provide fluidization state of the biomass, it is necessary to incorporate an inert material such as sand, glass beads, alumina [19–21].

It's noted that the use of such binary mixtures makes it possible to improve several aspects of the operation of equipment for thermochemical processing of solid fuels. On the one hand, finely dispersed inert material provides stable fluidization at lower flow rates of the fluidizing medium, and, on the other hand, such modes provide more intense gas-solid heat exchange in the equipment [20, 22].

However, the transition to a multicomponent (in particular, binary) mixture also means that the situation becomes more complicated. Obviously, to describe and predict such systems, it is necessary to understand the characteristics of each component. At the same time, it is necessary to establish the order of influence of one component on another and on the entire process as a whole. The above considerations mean that if we think in terms of mathematical modeling, then there is no need to change the approaches to mathematical modeling when working with mixtures; however, identifying model parameters when working with mixtures becomes more difficult. One can see that the existing numerical studies for biomass pyrolysis in fluidized-bed reactors are mainly based on Eulerian-Eulerian and Eulerian-Lagrangian multiphase flow models (DEM-CFD) [23-25]. Such models are based on the consideration of a conditionally infinitesimal volume, therefore they are very detailed and require the identification of a large number of parameters [23,26–31]. In this regard, in our study, the choice was made in favor of the concept of stochastic modeling based on the theory of Markov chains [32, 33]. In common case the device space in such models is not subject to decomposition into such small volumes as in DEM-CFD models [33-36]; however, if necessary, the level of detail can be increased, and the results obtained will be comparable to those obtained in DEM-CFD models [37].

The key aim of the present stage of the work is to construct a mathematical model of fluidization of inert material, identification of the most significant parameters of this model and their identification, as well as subsequent verification of the predictive capabilities of the model by comparing the modeling results with data from independent experiments.

Materials and methods

Theoretical methods. The transition from a continuous process representation to its description with a Markov chain model based on separation of operating volume of a reactor into *n* perfectly mixed cells of the length $\Delta x = H/n$

where H is the height of the reactor. The principal scheme of the proposed model design is shown in Fig. 1.

The property of the system that interests us is the content of particles (their number or mass) and gas content in each cell. It is convenient to organize all the specified contents in a state column vectors *S* (size $n \times 1$), then for a certain point in time the distribution of observable content along the height of the apparatus can be characterized as [32, 33, 36]:

$$\boldsymbol{S} = \begin{bmatrix} \boldsymbol{S}_1 \\ \boldsymbol{S}_2 \\ \dots \\ \boldsymbol{S}_N \end{bmatrix}.$$
(1)



Fig. 1. The principal scheme of the proposed Markov chain model of fluidization process

The total duration of the process observation can also be divided into finite

intervals of time Δt , and the current time can be presented as a sequence of discrete values $t_k = (k - 1)\Delta t$, where k is the time step number (k = 1, 2, ..., N; where N is the total number of observation time periods) [32, 33, 36].

During the *k*-th observation period, the state vector S^k changes and becomes S^{k+1} . The correlation between S^k and S^{k+1} can be described by the recurrent matrix formula [32, 33, 36]:

$$\mathbf{S}^{k+1} = \mathbf{P}^k \cdot \mathbf{S}^k,\tag{2}$$

where P is the transition probability matrix or transition matrix, which can be called the main operator of the Markov chain model [32, 33, 36].

In the case of a batch fluidization process, the specified matrix equality (2) can be adapted to construct models of gas flow and particle flow, represented as [36, 38, 39]:

$$\boldsymbol{S}_{\mathrm{s}}^{k+1} = \boldsymbol{P}_{\mathrm{s}}^{k} \cdot \boldsymbol{S}_{\mathrm{s}}^{k}, \qquad (3)$$

$$\boldsymbol{S}_{g}^{k+1} = \boldsymbol{P}_{g}^{k} \cdot \boldsymbol{S}_{g}^{k} + \boldsymbol{F}, \qquad (4)$$

where indexes 's' and 'g' assign the corresponding matrices to the solid and gas phases respectively, F is the vector of supply and discharge of fluidizing gas.

The vector F has two non-zero elements equal in modulus to the volume of gas supplied to the apparatus in one time interval Δt :

$$\boldsymbol{F} = \begin{bmatrix} \boldsymbol{q} \cdot \Delta t \\ \boldsymbol{0} \\ \dots \\ \boldsymbol{0} \\ -\boldsymbol{q} \cdot \Delta t \end{bmatrix}, \tag{5}$$

where q is the volumetric gas flow rate, $m^3 \cdot s^{-1}$.

The matrix P is the key operators of any Markov chain model. It consists of transition probabilities and can be constructed can be designed based on the following provisions: the *j*-th column of the matrix consists of probabilities related to the *j*-th cell, and the probability to transit into the *i*-th cell is placed in the *i*-th row of this column [36, 38, 39]. The book by A. Tamir [40] has brought much systematization into the field of general rules of Markov chain model construction, but the strategy of application of the theory to modeling in powder technology are examined and detailed in more recent works [32–34].

In the case of modeling a particular process a researcher have to solve two interrelated problems [32, 34]. The first is how to choose the structure of the model so that it best supports a qualitative description of the process, and the second is how to quantify the transition probabilities for the formation of the transition matrix. Depending on how both of these problems are solved, and how these solutions are coordinated with each other, quite diverse models of fluidized bed can be obtained [33, 36, 37, 39].

It should be noted that our work is generally focused on solving the second problem, since ultimately we need to have a predictive effective model capable of predicting a concrete process. However, it must be borne in mind that both problems are closely interrelated, since the issues of identifying model parameters depend on the adopted calculation scheme. The previous stages of work [36, 39, 41] have shown that the issues of parameter identification can, to a certain extent, be considered resolved. This doesn't mean that further work should not be carried out in this direction, but as a first approximation the convective-diffusion approach (one can read more about it in the works [33, 41]) for transition probabilities can be used. The obtained with way models are efficient to predict the expansion of the fluidized bed and the distribution of particles along its height [33, 36, 41].

In the considered models [36, 39, 41] under consideration the main attention is paid to identifying the probabilities of transition along a chain of cells of solid phase particles (elements of the matrix P). The convective-diffusion concept of forming matrices of transition probabilities involves separating the symmetrical (diffusion) component of the transfer probability and its asymmetrical part (convective). The transition matrix for the solid phase looks like follows [39]:

336

	$\left[1-v_i-d_i\right]$	d_{i}	0		0	0	
	$v_i + d_i$	$1 - v_i - 2 \cdot d_i$	$d_{_i}$	•••	0	0	
D _	0	$v_i + d_i$	$1 - v_i - 2 \cdot d_i$		0	0	(6)
1 _s –							, (0
	0	0	0		$1 - v_{n-1} - 2 \cdot d_{n-1}$	d_n	
	0	0	0		$v_{n-1} + d_{n-1}$	$1-d_n$	

where d is symmetrical part of the probability associated with random walk of particles (diffusion probability), v is asymmetrical part of the probability of particle transfer from a cell (convective probability).

The scheme for calculating these transition probabilities for the solid phase of a fluidized bed migration have been established and verified in previous works [36, 39, 41].

The diffusion probability is assumed to be related to a dispersion coefficient [33, 34, 41]:

$$d = D \frac{\Delta t}{\Delta x^2},\tag{7}$$

where the dispersion coefficient D can be quantified from the empirical relationship in the literature.

The following relation [42] is used in the present work to calculate the dispersion coefficient:

$$D = 0.051 \cdot \left(\frac{U_0}{U_{mf}}\right) \left(U_0 - U_{mf}\right)^{1.471},$$
(8)

where U_0 is a superficial gas velocity, U_{mf} is a minimum fluidization velocity.

The asymmetric part of the probability of particle transition from cell to cell is considered to be associated with the local gas velocity U_i in the *i*-th cell and particle settling velocity in the considered cell V_{si} [36, 41]:

$$v_i = \left| U_i - V_{si} \right| \frac{\Delta t}{\Delta x}.$$
(9)

The local gas velocity can be calculated as follows [36, 41]:

$$U_{i} = \frac{U_{0}}{1 - \pi \left(\frac{S_{s(i)}}{8S_{\max(i)}}\right)^{2/3}},$$
(10)

where S_s and S_{max} are the corresponding (*k*-th) moment of time and the maximum (for a dense bed state) values of the particle content in the cell.

The particle settling velocity V_s is considered to be related to the weight of the particle G as follows [36, 41]:

$$G = C_{d(i)} f \rho_g \frac{V_{s(i)}^2}{2} , \qquad (11)$$

where C_d is a drag force coefficient for identification of which, within the framework of this study, the following empirical formula was used [43]:

$$C_{d(i)} = \left(2.25 \operatorname{Re}_{i}^{-0.31} + 0.36 \operatorname{Re}_{i}^{0.06}\right)^{0.45},$$
(12)

where Re is the dimensionless Reynolds number.

Thus, the calculation scheme used assumes that convective transport probabilities are calculated for each computational domain separately, and probabilities of diffusion particle transfer are calculated for the entire fluidized bed as a whole. This calculation scheme is used quite often [36, 41], and good agreement between calculated predictions and experimental data is provided mainly by the choice of correlations for identifying model parameters.

Another traditional assumption for such cell models is the assumption that the gas moves from bottom to top in the ideal plug mode [36, 39, 41]. The transition matrix with such a movement has only two non-zero diagonals. The novelty of constructing the calculation scheme in this study is determined by the fact that the probability of gas backflow into previous cells is introduced into the model. This process is considered as stochastic and proportional to the diffusion of particles in the volume of the fluidized bed. In this case, the transition matrix already has three non-zero diagonals:

$$\boldsymbol{P}_{g} = \begin{bmatrix} 1 - u_{i} - p_{i} & p_{i} & 0 & \dots & 0 & 0 \\ u_{i} + p_{i} & 1 - u_{i} - 2 \cdot p_{i} & p_{i} & \dots & 0 & 0 \\ 0 & u_{i} + p_{i} & 1 - u_{i} - 2 \cdot p_{i} & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 1 - u_{n-1} - 2 \cdot p_{n-1} & p_{n} \\ 0 & 0 & 0 & \dots & u_{n-1} + p_{n-1} & 1 - p_{n} \end{bmatrix}, (13)$$

where u is a part of the gas transferred to the next cell in the chain and p is the proportion of gas transferred to neighboring cells due to random reasons.

Calculation of the fraction of gas displaced by the flow from the *i*-th cell is calculated as in previous works as a function of the local gas velocity U [36, 39]:

$$u_i = U_i \frac{\Delta t}{\Delta x} \,. \tag{14}$$

One of the assumptions of the model that determines the novelty is that gas is allowed to be thrown back into previous cells, and not just its ideal displacement forward along the chain. Obviously, such a view of the process increases the adequacy of the description, since the flow regime of the fluidizing medium in equipment with a fluidized bed is far from strictly laminar. In this study, the assumption was made that the random scatter of gas portions is associated with random walk of particles; accordingly, the following assumption was made:

$$p_i = k_u d_i, \tag{15}$$

where k_u is an empirical parameter of the proposed model.

Experimental setup. A schematic of the experimental setup is shown in Fig. 2. The main component of the setup was a cylindrical glass column with internal diameter 50 mm. There were 5 holes along the height of the apparatus, in which sensors (Testo-330) were installed to measure local gas flow rates. The sensor readings were taken during 10 minutes of the fluidization process at 1-minute intervals. The values obtained in this way for each height position were averaged over time. The averaged values were used to convert into solid phase concentration values according to the formula (10).

A narrow fraction of haydite particles was used as a bulk material for the experiments (fraction boundaries were limited using sieves 0.1 mm and 0.125 mm). The equivalent monofraction size was taken as 0.11 mm. The experiment was carried out at superficial gas velocities of 0.3 m/s, 0.4 m/s and 0.5 m/s (at each velocity was repeated three times and the results were averaged). In each individual ex-



Fig. 2. Installation diagram for the implementation of experimental research: 1 – gas distributor;
2 – gas velocity sensors;
3 – fluidized bed; 4 – glass column

periment, target measurements were taken during the first 10 minutes of the fluidization process. Then the fluidization process was stopped, the sensors were removed (to prevent its erosion), the holes were plugged, the air supply was restored, and fluidization continued for another 100 minutes. After this, the sensors were again placed in the apparatus and the measurements were repeated. Thus, the measurements were repeated after 110 minutes of fluidization of a sample of haydite particles in the apparatus. As a result, the distribution of particles along the height of the fluidized bed was established for each test sample of material for two time intervals (from 0 to 10 min and from 110 to 120 min). This repetition of the experiment was required because the particle size distribution of the product can change during fluidization process due to attrition [44–47].

Results and discussion

The obtained experimental results were used to achieve two goals. The first of these is the identification of model parameters. Fundamentally, the model has three parameters that require experimental identification, namely the particle drag coefficient C_d , the dispersion coefficient D, and the empirical coefficient k_u .

340

To calculate the first two indicated values, dependencies (8) and (12) were adopted, which have been used in the previous stages of the work [38, 39, 41, 48]. Thus, the fitting parameter was only the coefficient k_u characterizing the deviation of the gas flow characteristics from the ideal plug flow regime. To establish the value of this parameter experimental data at the gas superficial velocity of 0.4 m/s were used (the obtained values were used in modeling for other gas rates). For the fitting procedure itself, the least squares method was used to minimize the discrepancy between the calculated and experimental particle concentrations along the height of the apparatus. The coefficient values were sorted in steps of 0.1 for the range 0...1. The coefficient values were subject to enumeration in steps of 0.05 for the range $k_u = [0...1]$. On the Fig. 3 the comparison of the particle distributions obtained from the model (lines) and in the experiment (markers) at the superficial gas velocity of 0.4 m/s is shown.

The Fig. 3a allows comparing the experimental results with calculation results obtained under the assumption that the gas moves in the ideal plug mode. The Fig. 3a allows comparing the experimental results with calculation results obtained under the assumption that the gas moves has a stochastic component with $k_u = 0.35$ (at this value, the best agreement between the calculated and experimental data for this mode was obtained, so it was subsequently used for other fluidization modes within the framework of this study). As it can be seen from the Fig. 3, the inclusion of the parameter $k_u > 0$ in the model made it possible to more reliably describe the distribution of particles along the height of the fluidized bed.



Fig. 3. Distribution of local gas filtration velocity along the height of the fluidized bed apparatus (markers – experimental data; lines – calculated prediction) at superficial gas velocity 0.4 m/s: a – with model parameter $k_u = 0$; b – with model parameter $k_u = 0.35$

As can be seen from Fig. 4, the established value of the parameter $k_u > 0$ made it possible to describe more reliably the distribution of particles along the

height of the fluidized bed for other hydrodynamic regimes. Fig. 5 illustrates two trends. On the one hand, the model is well capable of predicting the distribution of gas velocities (and particles, respectively) with a known equivalent particle diameter. On the other hand, over time there appears to be a decrease in particle size due to attrition (after 110 minutes of fluidization, the equivalent particle size decreased from 1.1 to 1 mm). When substituting the last size into the model, the quality of prediction remains quite sufficient for engineering purposes; however, the gradual evolution of particle size is not taken into account in the model.



Fig. 4. Distribution of local gas filtration velocity along the height of the fluidized bed apparatus with model parameter $k_u = 0.35$ (markers – experimental data; lines – calculated prediction): a – at superficial gas velocity 0,3 m/s; b – at superficial gas velocity 0.5 m/s



Fig. 5. Distribution of local gas filtration velocity along the height of the fluidized bed apparatus with model parameter $k_u = 0.35$ and with superficial gas velocity 0,5 m/s (markers – experimental data: \Box – at first 10 minutes of fluidization process and \circ – after 110 minutes of fluidization process; lines – calculated prediction)

CONCLUSIONS

In the work, the model of fluidization of an ensemble of solid particles in an batch apparatus was constructed based on the mathematical approach of the theory of Markov chains. The model has a cellular structure, which makes it possible to describe the fluidization process by local parameters of its state. The movement of solid particles is considered in the model based on the convective-diffusion approach traditional for such models, which made it possible to identify the model parameters using dependencies known from the literature quite simply. At the same time, the novelty of the calculation scheme is ensured by the rejection of the traditional model of gas filtration in the ideal displacement mode and the introduction of a random scatter of gas portions between cells, proportional to the diffusion of particles with a proportionality coefficient k_{u} . Our own experiments on measuring local gas velocities in the laboratory unit with a fluidized bed made it possible to identify this parameter based on the consideration of one fluidization mode. The results of a comparison of calculation and experiment showed that the proposed calculation scheme increases the adequacy of the description of the fluidization process, and the identified value of the parameter k_{μ} can be used to describe other fluidization modes with a given bulk material. It has also been shown that during the fluidization process the material changes particle size distribution due to attrition. It was shown that the proposed model describes the velocity distribution for narrow fractions of expanded clay with sufficient accuracy; however, the very evolution of the particle size distribution (equivalent diameter of the monofraction) should be taken into account when modeling, which is a promising direction for the development of the proposed model.

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