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Methods of Nonequilibrium Statistical Mechanics in Models for Mixing Bulk Components

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Abstract

When describing the mechanics of the behavior of bulk materials during their mixing, a theoretical basis for the design of the specified equipment is formed. In recent years, the most well-known methods of modeling this process include the stochastic approach, in the framework of which models of the following types are actively developing: cell, managerial, with time series, energy, etc. Moreover, as a rule, predicting the quality of the finished mixture according to the selected criterion is achieved by using numerical calculation methods based on the generated cyber system. Of particular interest is the use of the energy method from the statistical mechanics of nonequilibrium processes due to the possibility of obtaining analytical simulation results. The paper describes the motion models of bulk components in rarefied flows, which are built on the basis of the energy method and take into account the main characteristics of the studied mixing process.

Keywords: apparatus, process, mixing, bulk material, rarefied flow, stochastic model

1. Introduction

Mixing of bulk materials belongs to the category of mechanical processes in the field of chemical technology in a variety of manufacturing enterprises, including paint and varnish, glass, construction, food, pharmaceutical, chemical, etc. The result of this technological operation is a loose mixture with a regulated degree of homogeneity, the quality of which is influenced by many factors. Moreover, factors that have a decisive influence on the quality of the final product can be conditionally divided into several types:

- Properties of components—physical, mechanical (particle-size distribution, tendency to adhesion, agglomeration, degree of moisture, etc.), and chemical.
- Features of the behavior of different-sized particles when moving in the working chamber of the apparatus under the established modes of its operation (segregation, classification).

- The features of mixing equipment are structural (the presence or absence of additional mixing elements, the nature of these elements, the dimensions of the working chamber, etc.) and operational (rotation speed of the apparatus elements, conveyor speed, consumable characteristics of materials).
- Features of the operating conditions of the mixer (dosing method, the presence or absence of a combination of mechanical, vibrational, and pneumatic types of mixing).

The multifactorial nature of the task of describing the behavior of particles of mixed components [1], as the basis for the formation of a cyber-physical system [2], requires, when choosing a method for modeling this mixing process, to take into account the possibility of evaluating the quality of the mixture [3], for example, from the standpoint of the average statistical deviation of the content of the key component in her samples. Moreover, analytical dependences (in comparison with numerical) between the heterogeneity coefficient of the resulting mixture and the selected parameter of the studied mixing process are preferred [4]. The significance of the formation of a theoretical platform for the design of mixing apparatuses based on system-structural analysis [5, 6] increases with the combination (sequential implementation) of several technological operations within the same apparatus [7]. The indeterminacy of the behavior of bulk components during their mixing allows us to choose stochastic approaches as appropriate modeling methods [8]. The aim of the work is to describe the main features of the application of the energy method [9, 10] from the statistical mechanics of nonequilibrium processes in modeling the motion of bulk components in rarefied flows during their mixing in various working volumes of chemical technology apparatuses, for example, constructions [11–13]

2. On modern methods of stochastic modeling of the process of mixing bulk solids

In contrast to the deterministic approach [14], when there is ambiguity between the given input parameters of the mathematical model of mixing bulk solids and the desired indicator of this process, in stochastic models [15, 16] there is ambiguity of correspondence between the initial and final states of the macrosystems of particles of each component. Currently, there is an active development of indeterministic methods built on various theoretical platforms, for example, statistical thermodynamics and information theory [15, 17]; principles of cybernetics [18, 19]; description of time series [20–22]; the A.A. Markov circuit theory [15, 23–29], including on the basis of the energy approach [9, 10] from the statistical mechanics of nonequilibrium processes, etc. Briefly Section 2 describes the main features of these methods of stochastic modeling.

2.1 General provisions of entropy-informational models of mixing bulk solids

The use of entropy-informational models is typical for the preparation of bulk mixtures with a ratio of components of 1: 100 or more [15, 17]. From the standpoint of information theory, the process of mixing granular media as a studied information system is characterized by an indicator of its disorder (uncertainty)—information entropy. At the same time, it is believed that obtaining all the useful information means bringing this system to zero uncertainty. On the other hand, this mixing operation can be considered as a thermodynamic system described by a

change in the Boltzmann entropy. A decrease in the latter leads to the transition of this system from a more probable state to a less probable one. Then, when applied to the process of mixing bulk materials, the maximum value of information entropy is determined by a logarithmic dependence on the number of components to be mixed with equal mass fractions and associated with the mixing efficiency parameter taking into account the specific fractions of each component in the selected sample of their many samples [17]. However, taking into account the peculiarities of the motion of the particles that make up the mixed components is difficult when using the specified entropy-information approach.

2.2 The main difficulties of using cybernetic models of granular media

Another variety of methods for mathematical modeling of the process of mixing bulk materials is the construction of models based on control theory [18, 19]. The cybernetic model describes the operation of the “input disturbance-mixer-output signal” system, in which the mixing apparatus plays the role of a “converter.” In this case, the residence time distribution function (DFID) of the particles of bulk components in the working volume of the apparatus is simulated depending on the response curve. Usually, perfect mixing is characterized by an exponential decrease of a given function from the specified argument with a mathematical expectation inversely proportional to the normalization coefficient. At the same time, the difficulties of using such a cybernetic model are associated with an experimental estimation of the model constants, scaling of the results obtained when the values of the structural and operating parameters of the process under study are changed, and the behavior of particles of mixed components is taken into account.

2.3 To the statement of the problem of identifying a trend class for a random mixing process

The next method for modeling the random process of mixing bulk solids relates to models of the theory of time series [20–22], which involve the construction of a set of correlation functions and other probabilistic characteristics. In this case, mixed flows of granular media are modeled as classes of elementary components of “trends” (components), depending on the time parameter and having a general systematically linear or nonlinear character, in contrast to another class of time series theory—the “seasonal component” with a periodically repeating component. In particular, superpositions of polynomial or trigonometric dependencies are used to ensure trend highlighting by fitting functions when modeling mixed flows with an explicit monotonic nonlinear component. However, the application of the theory of time series to the indicated technological operation of mixing bulk media involves not only solving the problem of identifying the model, in particular by the fitting method, but also forecasting with an appropriate estimate of the parameters of the random process. Note that the latter is achieved quite laboriously and the result is difficult to analyze for widespread use in the design of mixing equipment.

2.4 On the variety of descriptions of mixing using A.A. Markov chains

In the framework of the A.A. Markov circuit theory [23–27], there are many models for mixing bulk components, which are the basis for the design of mixers of various types and operating modes, with conditional classification in the form of the following stochastic descriptions: diffusion [28], kinetic [23], birth-death [15], etc. [29]. It is known that random processes are divided into two main classes from the standpoint of causality of the relationship between the states of the probability

system (events): (a) without correlations between events, when there is complete independence between the values, and (b) A.A. Markov processes, for which only the instantaneous states of the system are significant. In the latter case, the weight fraction of the key component of the granular mixture has the meaning of the probability density of a continuous random mixing process depending on the state and time parameter. For example, simulation of the share of a key component of a jump-like nature is used when layer-by-layer material splitting into cells or by postulating a matrix type of mass distribution of the mixed components with elements, as the probabilities of moving particles of materials from one selected area to another. In particular, in kinetic models [23], differential equations for the weight fractions of bulk components with spatiotemporal coordinates take into account their dispersion concentrations and mixing rate constants. In the birth-death models [15], these equations additionally contain a power-law dependence on spatial coordinates, and in diffusion models [28], there is a diffusion parameter along a given direction, and the influence of the acting force fields is taken into account. An active application of the A.A. Markov circuit method in his various interpretations with a cellular approach allows us to solve practical problems both with continuous and periodic operations of mixers. However, the difficulties that arise associated with the choice of the method of separation into cells and the calculation of the duration of the transition of the system to the boundary state are often solved by postulation. As a rule, two types of equations are used to describe continuous random mixing processes [25]: the Kolmogorov diffusion equation (e.g., for transverse and longitudinal displacements of component particles) and the Fokker-Planck kinetic equation for the probability density of the mixing process, as a consequence of the Chapman-Kolmogorov-Smoluchowski equation with a macrodiffusion coefficient and in the absence of a drift. In addition, cell models based on the Boltzmann equation [29] are known that allow the calculation of multidimensional combined processes of grinding, classification, and mixing of bulk materials. However, this modeling method in the case of forming torches of rarefied flows is difficult due to the complicated description of their behavior, for example, in a cylindrical coordinate system. Another variation in the use of A.A. Markov chains refers to the energy method [9, 10], which can be developed in two directions: with a description of the equilibrium (Ornstein-Uhlenbeck process) [4, 30, 31] and nonequilibrium [2, 32–34] distribution functions of the number of particles of mixed components in selected phase volume. Let us dwell on this method in more detail.

3. Features of the application of the energy method in stochastic modeling of the process of mixing bulk solids in rarefied flows

3.1 On the conditions for the formation of rarefied flows of bulk components in the working volumes of the apparatus

The principles of stochastic modeling of random processes are described in Yu. L. Klimontovich [9, 10], initially proved their effectiveness for equilibrium cases when studying shock processes in liquid-dispersed media [35], and then were successfully adapted in the analysis of the technological operation of separation of suspensions [36]. Studies of the random process of mixing bulk materials in different working volumes [11–13] with a set of additional mixing elements in the form of flexible bills [11], brushes [12], or elastic blades [13], as well as fenders [12, 13], showed the possibility of applying the energy method [9, 10]. This method of Yu. L. Klimontovich [9, 10] was used in two versions: for equilibrium [9] and

nonequilibrium [10] random processes for obtaining a bulk mixture in rarefied streams of constituent components.

The formation of these flows occurs when the bulk materials are scattered by mixing elements of the above types, which are fixed on the cylindrical surfaces of rotating drums, for example, along a helical line [11], on counter helical lines [12], and in tangent planes to these surfaces [13]. It should be noted that the main advantage of this mechanical method of mixing bulk solids is, first of all, the ability to control the effect of segregation, virtually eliminating its manifestations in the working volume of the apparatus by identifying and selecting rational ranges of changes in the design and operating parameters of the process under study. In this regard, the main task of modeling is to describe the mechanism of behavior of particles of bulk components when they are mixed in rarefied streams, followed by prediction of effective mixing conditions.

Consider the behavior of particles of mixed components ($i = \overline{1, n_k}$) in the working volume of the apparatus with the possibility of their scattering by mixing elements ($j = \overline{1, n_b}$) (Figure 1).

Let the grading composition by particle size of these components be known. The average values over fractions ($\nu = \overline{1, n_f}$) for the diameter and mass of particles of the components i are determined by the expressions $D_i = \sum_{\nu=1}^{n_f} d_{i\nu}$; $M_i = \sum_{\nu=1}^{n_f} m_{i\nu}$. It is believed that the speed of their centers of mass has correspondingly components (V_{xij}, V_{yij}) and ($V_{rij}, V_{\theta ij}$) in Cartesian (x, y) and polar (r, θ) coordinate systems in the projection onto the plane of the cross section of a mixing drum rotating at an angular speed ω . The choice of centers of coordinate systems depends on the geometry of the working area of the mixing apparatus (Figure 1).

Let random scattering by mixing elements ($j = \overline{1, n_b}$) specified particles from sets ($i = \overline{1, n_k}$) can occur according to two schemes: (A) in the absence of their collisions, when particle motion is observed in practically combined flows i with one direction of distribution, and (B) in the presence of collisions of particles from intersecting flows i . Conditional images of the described circuits A and B are presented at Figure 2 in the case of mixing two streams of bulk components ($i = 1, 2$) from one (Figure 2A) and two (Figure 2B) point sources C_0 for circuit A and points C_1, C_2 for Scheme B.

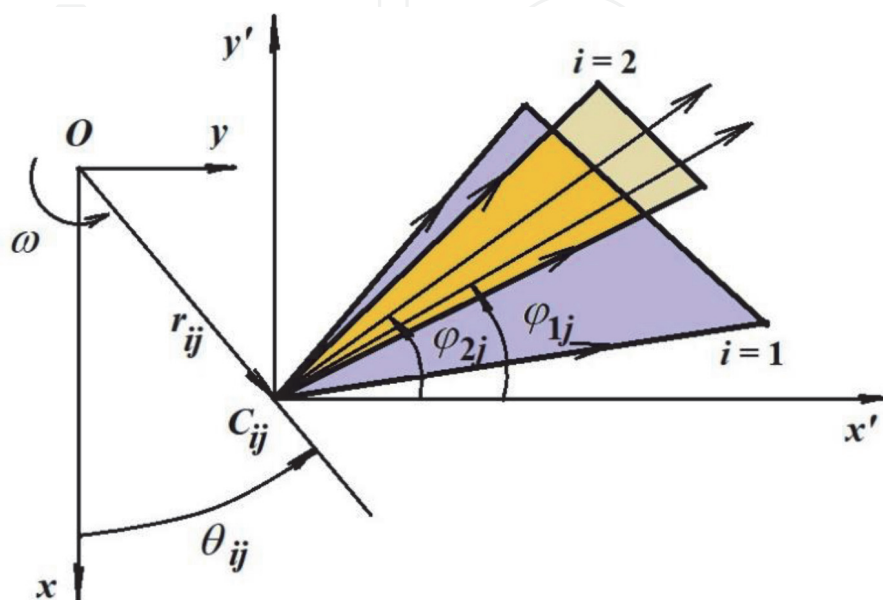


Figure 1.
 Conditional coordinate system selection scheme.

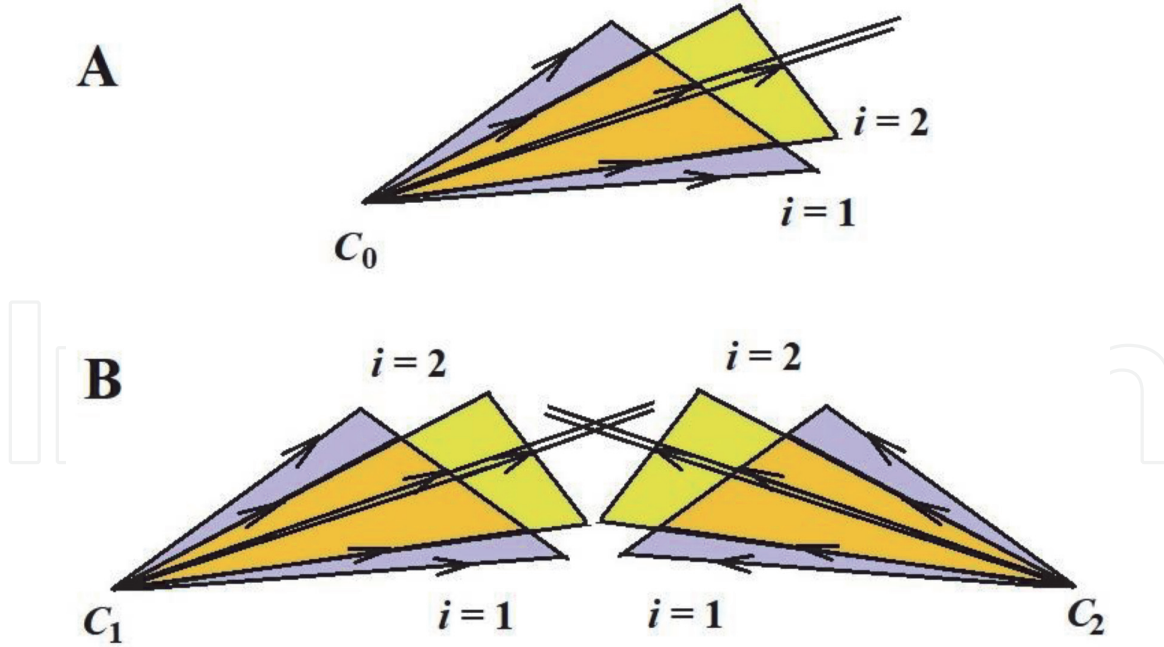


Figure 2. Scattered images of loose components ($i = 1, 2$) sources of $C_\varepsilon, \varepsilon = 0, 1, 2$: (A) scheme A; (B) scheme B.

Each Scheme A and B needs its own stochastic description, taking into account the presence or absence of large-scale fluctuations in the states of the macrosystem, as a set of particles for a component i .

3.2 The case of combining rarefied flows of bulk materials

Scheme A (**Figure 2A**) implies the constancy of the average energy value over the Gibbs ensemble for each macrosystem (bulk component i) in the approximation of the same microsystems (particles of one component i). Coordinate (x_{ij}, y_{ij}) and impulse $(M_{ij}V_{xij}, M_{ij}V_{yij})$ component mass centers i after spreading with a mixing element j in this case play the role of Hamilton parameters. Then, the state of the macrosystem i obeys the principle of maximum entropy, i.e., an increase in entropy characterizes the evolution of a macrosystem to an equilibrium state, and its conservation means the achievement of this equilibrium. Therefore, the random process of mixing granular media according to Scheme A is characterized by instantaneous states of macrosystems i and can be modeled as a homogeneous and stationary process A.A. Markov [9, 10, 25]. In addition, taking into account the approximations of the absence of large-scale particle collisions, a continuous, homogeneous, stationary random Gaussian process is considered. This process obeys the Ornstein-Uhlenbeck formalism [9, 35]; then when choosing an element of the phase volume in the Cartesian and polar coordinate systems

$$d\Omega_{ij} = dV_{xij}dV_{yij} = \omega^2 r_{ij} dr_{ij} d\theta_{ij} \quad (1)$$

Fokker-Planck type kinetic equation for distribution functions $U_{Aij}(V_{xij}, V_{yij}, t)$ or $u_{Aij}(r_{ij}, \theta_{ij}, t)$ for the state of macrosystems of particles of mixed components, it has diffusion and drift components. According to Eq. (1) and relations from [34] for phase variables in various coordinate systems

$$\partial\theta_{ij}/\partial V_{xij} = -(\omega r_{ij})^{-1} \sin \theta_{ij}, \partial\theta_{ij}/\partial V_{yij} = (\omega r_{ij})^{-1} \cos \theta_{ij} \quad (2)$$

we have the following forms of the Fokker-Planck equation for Scheme A of mixing bulk solids (**Figure 2A**):

$$\frac{\partial U_{Aij}(V_{xij}, V_{yij}, t)}{\partial t} = D_{1ij} \frac{\partial^2 U_{Aij}}{\partial V_{xij}^2} + D_{2ij} \frac{\partial^2 U_{Aij}}{\partial V_{yij}^2} + q_{1ij} \frac{\partial(V_{xij} U_{Aij})}{\partial V_{xij}} + q_{2ij} \frac{\partial(V_{yij} U_{Aij})}{\partial V_{yij}}, \quad (3)$$

$$\begin{aligned} \frac{\partial u_{Aij}(r_{ij}, \theta_{ij}, t)}{\partial t} = & D_{1ij} \left\{ \cos^2 \theta_{ij} \frac{\partial^2 u_{Aij}}{\partial r_{ij}^2} + \frac{\sin^2 \theta_{ij}}{r_{ij}} \left[\frac{\partial u_{Aij}}{\partial r_{ij}} + \frac{1}{r_{ij}} \frac{\partial^2 u_{Aij}}{\partial \theta_{ij}^2} \right] - \frac{\sin 2\theta_{ij}}{r_{ij}} \times \right. \\ & \left. \times \left[\frac{\partial^2 u_{Aij}}{\partial r_{ij} \partial \theta_{ij}} - \frac{1}{r_{ij}} \frac{\partial u_{Aij}}{\partial \theta_{ij}} \right] \right\} + D_{2ij} \left\{ \sin^2 \theta_{ij} \frac{\partial^2 u_{Aij}}{\partial r_{ij}^2} + \frac{\cos^2 \theta_{ij}}{r_{ij}} \left[\frac{\partial u_{Aij}}{\partial r_{ij}} + \frac{1}{r_{ij}} \frac{\partial^2 u_{Aij}}{\partial \theta_{ij}^2} \right] + \right. \\ & \left. \frac{\sin 2\theta_{ij}}{r_{ij}} \left[\frac{\partial^2 u_{Aij}}{\partial r_{ij} \partial \theta_{ij}} - \frac{1}{r_{ij}} \frac{\partial u_{Aij}}{\partial \theta_{ij}} \right] \right\} + (q_{1ij} + q_{2ij}) u_{Aij} + q_{1ij} \left[\cos \theta_{ij} \frac{\partial u_{Aij}}{\partial r_{ij}} - \frac{\sin \theta_{ij}}{r_{ij}} \frac{\partial u_{Aij}}{\partial \theta_{ij}} \right] + \\ & + q_{2ij} \left[\sin \theta_{ij} \frac{\partial u_{Aij}}{\partial r_{ij}} - \frac{\cos \theta_{ij}}{r_{ij}} \frac{\partial u_{Aij}}{\partial \theta_{ij}} \right]. \end{aligned} \quad (4)$$

In Eq. (3), four designations are accepted: D_{1ij} , D_{2ij} , diffusion parameters in the directions of the vectors of the Cartesian velocity components; q_{1ij} , q_{2ij} , drop rates by the mixing element j component particles i ; and t , time parameter.

Besides, in Eq. (4) it is advisable to lead to an energy representation regarding the distribution function $u_{Aij}(E_{ij}, t)$:

$$\frac{\partial u_{Aij}(E_{ij}, t)}{\partial t} = \Psi_{A0ij} \left[\frac{\partial}{\partial E_{ij}} \left(E_{ij} \frac{\partial u_{Aij}}{\partial E_{ij}} \right) + \frac{1}{E_{A0ij}} \frac{\partial(E_{ij} u_{Aij})}{\partial E_{ij}} \right], \quad (5)$$

where E_{ij} is the energy of the stochastic motion of the particles of the component i after spreading with a mixing element j ; t_0 is the time moment, when there was stochastization of the macrosystems of the particles of each component, i.e., particle motion paths and solutions of dynamic equations acquire a probabilistic nature; and $E_{A0ij} = E_{ij}(t_0)$ is the stationary value of energy E_{ij} at the time of stochastization t_0 . The semantic load of the parameter $\Psi_{A0ij} \equiv (dE_{ij}/dt)|_{t_0}$ in Eq. (5) corresponds to the flow of energy at the time of stochastization of each of these macrosystems. According to the data of [34], the species in Eqs. (4) and (5) allow us to take the approximation $\Psi_{A0ij} = 4\lambda_{1ij}D_{1ij} = 4\lambda_{2ij}D_{2ij}$, if the energy of the stochastic motion of the particles of the component i in accordance with Eq. (1) is defined by the expression:

$$E_{ij} = \lambda_{1ij} V_{xij}^2 + \lambda_{2ij} V_{yij}^2 \quad (6)$$

where λ_{1ij} , λ_{2ij} are the coefficients depending on the structural and operational parameters of the apparatus, as well as the physico-mechanical properties of the mixed bulk materials. The stationary solution of the kinetic equation of the Fokker-Planck type in Eq. (5) subject to Eq. (6) represented in the form of an exponential dependence on energy E_{ij} :

$$u_{Aij}(E_{ij}, t_0) = \alpha_{Aij} \exp(-E_{ij}/E_{A0ij}) \quad (7)$$

where the normalization parameter α_{Aij} according to Eq. (1) depends on the selected element of the phase volume and is calculated using the equation:

$$\int_{\Omega_{ij}} u_{Aij} d\Omega_{ij} = 1.$$

Thus, the choice of Scheme A (**Figure 2A**) leads to the following form for $u_{1Aij}(\varphi_j)$, differential particle number distribution function N_{Aij} each component i after spreading with a mixing element j by the selected parameter, for example, the spreading angle φ_j (**Figure 1**), whose reference is determined by the coordinate system used and the geometry of the working volume of the apparatus

$$u_{1Aij}(\varphi_j) = (dN_{Aij}/d\varphi_j)/N_{Aij}, \quad (8)$$

if the calculation of the number of particles in the phase volume element $d\Omega_{ij}$ is performed by the formula:

$$dN_{Aij} = \alpha_{1Aij} \exp(-E_{ij}/E_{1A0ij})d\Omega_{ij}. \quad (9)$$

In this form $u_{1Aij}(\varphi_j)$ from Eq. (7) allows to describe $w_{1Ai}(\varphi_j)$ —full functional dependencies for the distribution of the number of particles of the component i after scattering by all deformed mixing elements of the drum according to the selected characteristic of the mixing process φ_j :

$$w_{1Ai}(\varphi_j) = \prod_{j=1}^{n_b} u_{1Aij}(\varphi_j). \quad (10)$$

So, for use $w_{1Ai}(\varphi_j)$ in Scheme A (**Figure 2A**), two sets of parameters need to be calculated: normalization parameter α_{1Aij} and stationary value of the energy of stochastic particle motion of the component i after spreading with a mixing element j at the time of stochastization E_{1A0ij} .

3.3 The case of crossing rarefied flows of bulk components

Scheme B (**Figure 2B**) for the random process of mixing bulk solids has a number of significant differences. Taking into account the principles of the energy method of stochastic modeling [10], it is believed that in the case of crossing rarefied flows of loose components, large-scale fluctuations of the states of the corresponding macrosystems are observed, such as collisions of particles that are scattered by two sources symmetrically located at points C_1, C_2 . In this case, the small-scale fluctuations of the states of these macrosystems of particles related to their collisions during scattering from each source separately, i.e., in combined rarefied streams. Then, the macrosystems of particles are not energetically closed, and to describe the evolution of their states, it is proposed to apply the formalism of random sources of Langevin in the Fokker-Planck kinetic equation according to the energy approach from [10]. In this case, the ordering of the states of the macrosystems of the components is characterized by the S-theorem for the Lyapunov function, given by the change in the values of the Boltzmann-Gibbs-Shannon entropy for different states of each macrosystem when the energy index is averaged. The decisive role in finding the control parameters of the random mixing process to achieve the state of ordering of the component macrosystems belongs to the operation of renormalization of the Boltzmann-Gibbs-Shannon entropy.

Therefore, with the introduction g_{1ij}, g_{2ij} —collision coefficients as large-scale fluctuations—the presence of Langevin sources leads to the following changes in the notation of the Fokker-Planck kinetic equation with respect to the distribution

function $U_{Bij}(V_{xij}, V_{yij}, t)$ or $u_{Bij}(r_{ij}, \theta_{ij}, t)$ in contrast to the species in Eq. (3) according to Eq. (2):

$$\begin{aligned} \frac{\partial U_{Bij}(V_{xij}, V_{yij}, t)}{\partial t} = & D_{1ij} \frac{\partial^2 U_{Bij}}{\partial V_{xij}^2} + D_{2ij} \frac{\partial^2 U_{Bij}}{\partial V_{yij}^2} + q_{1ij} \frac{\partial(V_{xij} U_{Bij})}{\partial V_{xij}} + q_{2ij} \frac{\partial(V_{yij} U_{Bij})}{\partial V_{yij}} \\ & + g_{1ij} \frac{\partial(V_{xij} E_{ij} U_{Bij})}{\partial v_{xij}} + g_{2ij} \frac{\partial(V_{yij} E_{ij} U_{Bij})}{\partial v_{yij}}, \end{aligned} \quad (11)$$

$$\begin{aligned} \frac{\partial u_{Bij}(r_{ij}, \theta_{ij}, t)}{\partial t} = & D_{1ij} \left\{ \cos^2 \theta_{ij} \frac{\partial^2 u_{Bij}}{\partial r_{ij}^2} + \frac{\sin^2 \theta_{ij}}{r_{ij}} \left[\frac{\partial u_{Bij}}{\partial r_{ij}} + \frac{1}{r_{ij}} \frac{\partial^2 u_{Bij}}{\partial \theta_{ij}^2} \right] - \frac{\sin 2\theta_{ij}}{r_{ij}} \times \right. \\ & \left. \times \left[\frac{\partial^2 u_{Bij}}{\partial r_{ij} \partial \theta_{ij}} - \frac{1}{r_{ij}} \frac{\partial u_{Bij}}{\partial \theta_{ij}} \right] \right\} + D_{2ij} \left\{ \sin^2 \theta_{ij} \frac{\partial^2 u_{Bij}}{\partial r_{ij}^2} + \frac{\cos^2 \theta_{ij}}{r_{ij}} \left[\frac{\partial u_{Bij}}{\partial r_{ij}} + \frac{1}{r_{ij}} \frac{\partial^2 u_{Bij}}{\partial \theta_{ij}^2} \right] + \right. \\ & \left. \frac{\sin 2\theta_{ij}}{r_{ij}} \left[\frac{\partial^2 u_{Bij}}{\partial r_{ij} \partial \theta_{ij}} - \frac{1}{r_{ij}} \frac{\partial u_{Bij}}{\partial \theta_{ij}} \right] \right\} + (q_{1ij} + q_{2ij}) u_{Bij} + q_{1ij} \left[\cos \theta_{ij} \frac{\partial u_{Bij}}{\partial r_{ij}} - \frac{\sin \theta_{ij}}{r_{ij}} \frac{\partial u_{Bij}}{\partial \theta_{ij}} \right] + \\ & + q_{2ij} \left[\sin \theta_{ij} \frac{\partial u_{Bij}}{\partial r_{ij}} - \frac{\cos \theta_{ij}}{r_{ij}} \frac{\partial u_{Bij}}{\partial \theta_{ij}} \right] + g_{1ij} \left[\cos \theta_{ij} \frac{\partial(E_{ij} u_{Bij})}{\partial r_{ij}} - \frac{\sin \theta_{ij}}{r_{ij}} \frac{\partial(E_{ij} u_{Bij})}{\partial \theta_{ij}} \right] + \\ & + g_{2ij} \left[\sin \theta_{ij} \frac{\partial(E_{ij} u_{Bij})}{\partial r_{ij}} - \frac{\cos \theta_{ij}}{r_{ij}} \frac{\partial(E_{ij} u_{Bij})}{\partial \theta_{ij}} \right]. \end{aligned} \quad (12)$$

Similar to Eq. (5), it is convenient in the future to use the energy representation of the Fokker-Planck equation with respect to the distribution function $u_{Bij}(E_{ij}, t)$

$$\frac{\partial u_{Bij}(E_{ij}, t)}{\partial t} = (\Psi_{B0ij} \Psi_{fij})^{1/2} \left[\frac{\partial}{\partial E_{ij}} \left(E_{ij} \frac{\partial u_{Bij}}{\partial E_{ij}} \right) + \frac{1}{E_{B0ij}} \frac{\partial(E_{ij} u_{Bij})}{\partial E_{ij}} + \frac{1}{E_{fij}^2} \frac{\partial(E_{ij}^2 u_{Bij})}{\partial E_{ij}} \right], \quad (13)$$

where $E_{B0ij} = E_{ij}(t_0)$; $\Psi_{B0ij} \equiv (dE_{ij}/dt)|_{t_0}$ have the same physical meaning as in Eq. (5); $E_{fij} \equiv E_{ij}(\Delta t)$, particle energy loss of each component i after spreading with a mixing element j in collisions, as macroscale fluctuations of the states of the system over a period of time Δt ; and $\Psi_{fij} \equiv (dE_{ij}/dt)|_{\Delta t}$, changes in these energy losses over Δt .

In particular, on the basis of the approach [10], the parameters were identified in [34] $\mu_{ijk}, k = 0, 1, 2, 3$ for the random process of mixing bulk materials: manager $\mu_{ij0} = (\Psi_{B0ij} \Psi_{fij})^{1/2} / E_{B0ij}$ and optimizing $\mu_{ij1} = (\Psi_{B0ij} \Psi_{fij})^{1/2}$; $\mu_{ij2} = (\Psi_{B0ij} \Psi_{fij})^{1/2} / E_{B0ij}^2$; $\mu_{ij3} = \Psi_{fij} / E_{fij}$. Note that, if necessary, estimates of diffusion parameters in the directions of the vectors of the Cartesian velocity components D_{1ij}, D_{2ij} can be used through the method proposed in the work [37].

In addition, the main stages of the formation of rarefied flows corresponding to various states of component macrosystems were identified in [34]:

- Smoothing out small-scale fluctuations of the states of macrosystems during the dropping of particles from deformed mixing elements in the region of combining rarefied flows, when $\mu_{ij0} = 0$ and $\Psi_{B0ij} \ll 1$ rightly for Eq. (7)
- Nucleation of large-scale fluctuations in the states of macrosystems of mixed components at the boundary of the regions of overlapping and crossing of their

rarefied flows, if the state of the regeneration threshold is realized $\mu_{ij0} = \mu_{ij3}$ with a solution of the form $u_{ABij} = \alpha_{ABij} \exp \left[-E_{ij}^2 (2E_{AB0ij})^{-1} \right]$ for Eq. (13)

- An increase in energy losses with an increasing intensity of large-scale fluctuations in the states of macrosystems of mixed components i in the area of crossing of their rarefied flows, when the regeneration mode can be implemented, a transition to a new stationary state in a certain range of variation of the control parameter μ_{ij0}

In the latter case, the solution Eq. (13) corresponds to the regime of advanced regeneration, when the relations $\mu_{ij0}\mu_{ij3}^{-1} < < 1$ and $\mu_{ij1}\mu_{ij2}\mu_{ij0}^{-2} < < 1$ are true

$$u_{Bij} = \alpha_{Bij} \exp \left[-E_{ij}/E_{B0ij} + E_{ij}^2 / (2E_{fij}) \right] \quad (14)$$

where α_{Bij} is the normalization parameter taking into account Eq. (1) determined from the equation $\int_{\Omega_{ij}} u_{Bij} d\Omega_{ij} = 1$.

Therefore, the choice of Scheme B (**Figure 2B**) allows according to Eq. (14) to build dependencies $u_{1Bij}(\varphi_j)$ for differential distribution functions of the number of particles N_{Bij} of each component i after spreading by the mixing element j , for example, by the spread angle φ_j (**Figure 1**), in this case, similar to Eq. (8), (9) we have

$$u_{1Bij}(\varphi_j) = (dN_{Bij}/d\varphi_j) / N_{Bij}, \quad (15)$$

$$dN_{Bij} = \alpha_{1Bij} \exp(-E_{ij}/E_{1B0ij}) d\Omega_{ij}. \quad (16)$$

Then, when describing the complete differential distribution functions of the number of particles of the components after scattering by all deformed mixing elements of the drum in the corner φ_j , as in Eq. (10), dependencies are used

$u_{1Bij}(\varphi_j)$ from Eq. (15):

$$w_{1Bi}(\varphi_j) = \prod_{j=1}^{n_b} u_{1Bij}(\varphi_j) M_i V_{r\theta_{ij}}^2 / 2L_{ij}^2 / (2I_i) k_u \theta_{ij}^2 / 2. \quad (17)$$

So for analysis $u_{1Bij}(\varphi_j)$ in Scheme B (**Figure 2B**), it is necessary to carry out the calculation of three sets of parameters: normalization parameter α_{1Bij} ; stationary value of the energy of stochastic motion of the particles of the component i after spreading with mixing element j at the time of stochastization E_{1B0ij} ; and particle energy loss of each component after interacting with the mixing element j in interparticle collisions E_{fij} .

4. The results of stochastic modeling of the motion of bulk components in rarefied flows during their mixing

We give some examples of the application of stochastic mixing models built on the basis of the energy method [9, 10] according to the two motion schemes of rarefied flows of bulk components considered in paragraph 3. Initially, we set the type of energy of the stochastic motion of particles of mixed components $i = 1, 2$

after spreading with a mixing element j . As the working volumes of the mixing apparatus, we will choose the elements of a number of designs, for example, [11–13]. In all three cases, rarefied flows are ensured by the spreading of particles of bulk materials i with the help of mixing elements fixed on rotating drums in the form of flexible bills located along a helical line [11]; brushes installed with multidirectional screw coils [12]; and elastic blades in tangent planes to the surface of the drum [13]. In designs [11, 13], the mixing process is carried out on a movable tape, in the apparatus [12]—on the tray of gravity equipment. The geometry features of drum mixing devices [11, 13] allow the mixing process to be carried out according to Scheme A when combining rarefied flows (**Figure 2A**) and for the apparatus [12] according to Scheme B when they are crossed (**Figure 2B**). Let the energy E_{ij} consists of three components, taking into account the translational movement of the particle of the component in the transverse plane of the cross section of the mixing drum i together with its center of mass ($M_i V_{r\theta ij}^2/2$), rotational motion relative to it ($L_{ij}^2/(2I_i)$), and elastic interaction with a deformed mixing element ($k_u \theta_{ij}^2/2$). Here, in addition to the notation from paragraph 2, the following are additionally introduced: L_{ij} , random moments of impulses; I_i , axial moments of inertia; and k_u , angular stiffness of the mixing element. According to Eq. (1), (6) dependence $E_{ij}(r_{ij}, \theta_{ij})$ with averaged values $\theta_{im} = (1/n_b) \sum_{j=1}^{n_b} \theta_{ij}$ by the number of deformed mixing elements has a general view $E_{ij} = \varepsilon_{1ij}(\theta_{im})r_{ij}^2 + \varepsilon_{2}\theta_{ij}^2$.

Without dwelling in detail on the analysis of the features of each model for the indicated types of mixing apparatuses, we present some of their results to illustrate the possibility of a preliminary assessment of the effectiveness of the process of mixing bulk components. Note that the model parameters are the design and operating parameters of the mixer, as well as the physical and mechanical characteristics of the working media and mixing elements (in particular, angular stiffness $k_u = 1.6 \times 10^{-4} \text{ kg} \times \text{m/rad}$). The working bulk materials include natural sand GOST 8736-93 ($D_i = 1.5 \times 10^{-4} \text{ m}$, $\rho_i = 1.525 \times 10^3 \text{ kg/m}^3$) and soda ash GOST 5100-85 ($D_i = 1.75 \times 10^{-4} \text{ m}$, $\rho_i = 1.08 \times 10^3 \text{ kg/m}^3$). The calculations were performed using the software xwMaxima18.02.0; for visualization, the gnuplot 5.2 environment was used.

An example of the results of stochastic modeling of obtaining a granular mixture in the presence of natural sand GOST 8736-93 in combined rarefied flows (Scheme A; **Figure 2A**) [4, 30, 31] when they are scattered from a movable belt by flexible bills located along a helix on the surface of a rotating drum in a mixer [11] on **Figure 3** shows a family of surfaces for dependencies $u_{1A2j}(\varphi_j, \Delta)$ and $w_{1A2}(\varphi_j, \Delta)$ according to Eq. (1) (7)-(10). An analysis of these functions shows a significant effect of the complex parameter $\Delta = h_0/l_b$, characterizing the degree of deformation of flexible bill length l_b after leaving the height gap h_0 between the tape and the drum on the distribution of the number of component particles ($i = 2$) after elastic interaction with the bills j . Therefore, in addition to the operational parameter (angular velocity of rotation of the drum), there are other significant factors affecting the process under study. As was shown earlier [4, 30, 31], the design parameters of the apparatus can be attributed to such factors: step of screw winding h_s for the flexible bill. Note that the radius also belongs to the set of design parameters r_b and length L_b of drum. The classes of parameters of this mixing process are discussed in more detail in [4, 30, 31].

An example of the implementation of the conditions for mixing bulk components with crossed rarefied streams (Scheme B; **Figure 2B**) is the operation of the gravitational apparatus when scattering mixed materials from its tray with brush elements mounted with multidirectional screw windings on a rotating drum [12].

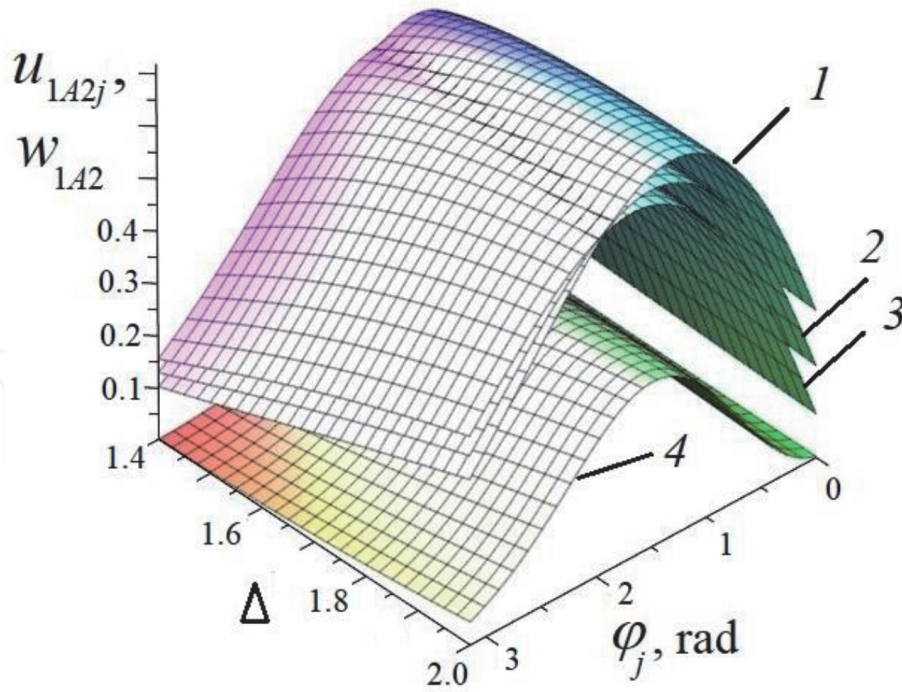


Figure 3.

Dependencies $u_{1A2j}(\varphi_j, \Delta), w_{1A2}(\varphi_j, \Delta)$ for natural sand GOST 8736-93 ($i = 2$) when scattering from a movable belt with flexible bills located along a helix on the surface of a rotating drum (Scheme A): $\omega = 52.36 \text{ c}^{-1}; h_s = 1.6 \times 10^{-2} \text{ m}; r_b = 3.0 \times 10^{-2} \text{ m}; L_b = 1.85 \times 10^{-1} \text{ m}; l_b = 4.5 \times 10^{-2} \text{ m}; 1, j = 1; 2, j = 2; 3, j = 3$ for $u_{1A2j}(\varphi_j, \Delta)$; and 4, for $w_{1A2}(\varphi_j, \Delta)$.

According to the stochastic modeling performed by the authors [2, 32–34] in accordance with Eq. (1), (14)–(17), we give the dependencies $u_{1B2j}(\varphi_j, \Delta)$ for soda ash GOST 5100-85 ($i = 2$) (Figure 4).

In this case, a detailed analysis of the simulation results given in [2, 34] revealed the conditions for the effective mixing of bulk components, as a result of the convergence of the spreading angles corresponding to the extrema for each working solid-dispersed medium. The obtained dependencies for distribution functions

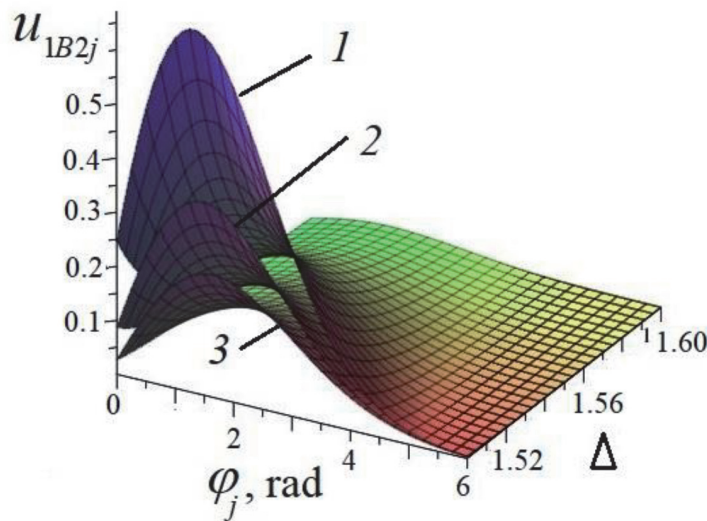


Figure 4.

Dependencies $u_{1B2j}(\varphi_j, \Delta)$ for soda ash GOST 5100-85 ($i = 2$) when scattering the gravitational apparatus from the tray with brush elements installed with multidirectional screw windings on a rotating drum (scheme B): $\omega = 52.36 \text{ c}^{-1}; h_s = 1.6 \times 10^{-2} \text{ m}; r_b = 3.0 \times 10^{-2} \text{ m}; L_b = 1.85 \times 10^{-1} \text{ m}; l_b = 4.5 \times 10^{-2} \text{ m}; 1, j = 1; 2, j = 2; \text{ and } 3, j = 3$.

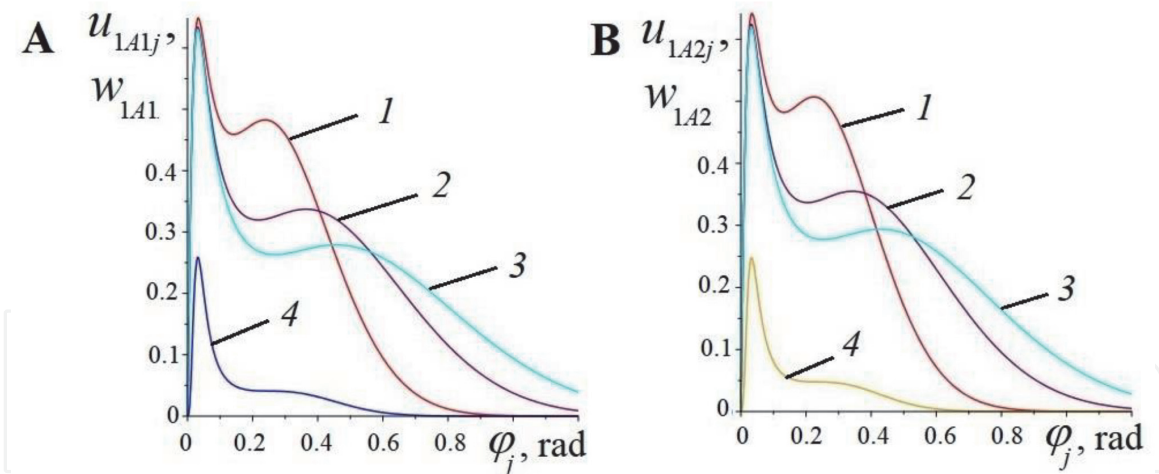


Figure 5.
 Dependencies when scattering loose components from a movable belt with elastic blades in tangent planes to the surface of the mixing drum (scheme A): A, soda ash GOST 5100-85 ($i = 1$); B, natural sand GOST 8736-93 ($i = 2$); $\omega = 52.36 \text{ c}^{-1}$; $r_b = 3.0 \times 10^{-2} \text{ m}$; $L_b = 1.85 \times 10^{-1} \text{ m}$; $l_b = 4.5 \times 10^{-2} \text{ m}$; 1, $j = 1$; 2, $j = 2$; 3, $j = 3$ for $u_{1Aij}(\varphi_j)$; and 4, for $w_{1A2}(\varphi_j)$.

$u_{1A2j}(\varphi_j, \Delta)$ and $u_{1B2j}(\varphi_j, \Delta)$ shown on **Figures 3** and **4** have a general character with a pronounced maximum of the operating ranges of parameter changes and are confirmed experimentally [2, 34] with a relative error not exceeding 18% for scheme A and 12% for scheme B.

Let us show that in the case of scattering of loose components from the moving tape by elastic blades fixed in tangent planes to the surface of the mixing drum [13], the result of the implementation of scheme A (**Figure 2A**, **Figure 5**) may not be inferior in its efficiency to the operation of scheme B (**Figure 2B**) for rational choice of design and operational parameters of the device.

In particular, when modeling in the plane of the cross section of the drum the equations of motion of the end points of the elastic blades using the Archimedes spiral equation, the application in Eq. (1) (7)-(9) allows you to get dependencies

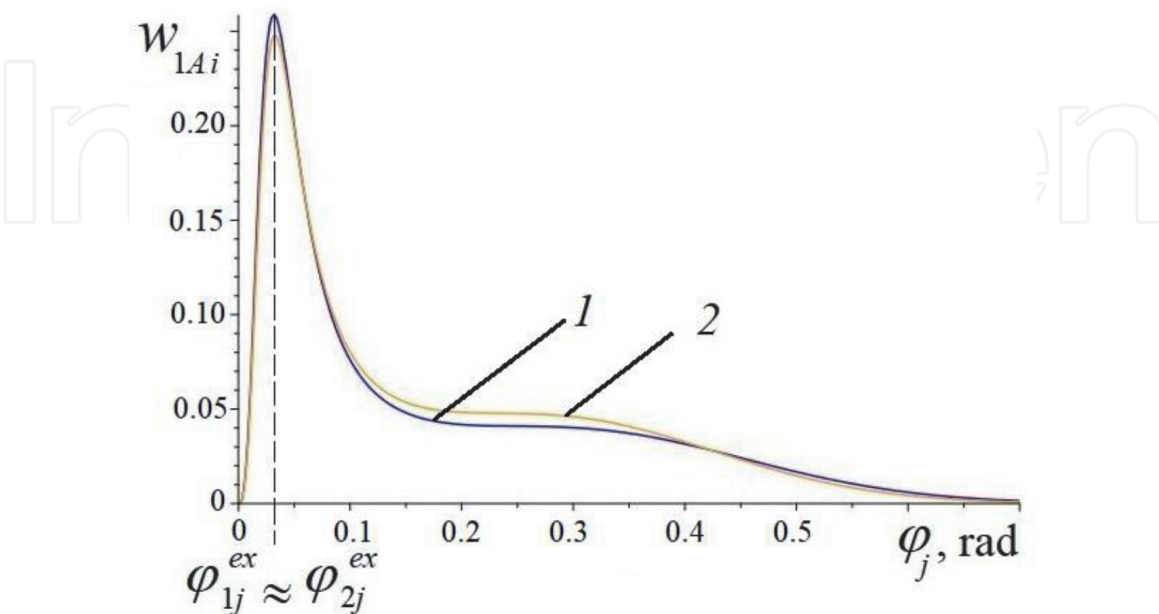


Figure 6.
 Comparison of dependencies when scattering loose components from a moving tape with elastic blades in tangent planes to the surface of the mixing drum (scheme A): 1, soda ash GOST 5100-85 ($i = 1$); 2, natural sand GOST 8736-93 ($i = 2$); $\omega = 52.36 \text{ c}^{-1}$; $r_b = 3.0 \times 10^{-2} \text{ m}$; $L_b = 1.85 \times 10^{-1} \text{ m}$; $l_b = 4.5 \times 10^{-2} \text{ m}$.

$u_{1Aij}(\varphi_j)$ or soda ash GOST 5100-85 (**Figure 5A**) and natural sand GOST 8736-93 (**Figure 5B**). The presented families of curves show that the bulk of each bulk material when they are mixed is scattered with elastic blades at the initial angles of rotation of the drum (see the first burst on the graphs 1–3; **Figure 5A**, **Figure 5B**). Moreover, there is the possibility of subsequent self-cleaning of the deformed mixing elements when the angular coordinate of the ends is less than 0.758 rad (see the second surge in the charts 1–3; **Figure 5A**, **Figure 5B**). Benchmarking dependencies $w_{1Ai}(\varphi_j)$ (**Figure 6**) showed preferably the cleaning of the blades at the initial stage of restoration of their geometric shape.

In addition, according to **Figure 6**, the conditions for efficient mixing of bulk components are observed. $i = 1, 2$ due to the approach of not only extreme angular values $\varphi_{1j}^{ex} \approx \varphi_{2j}^{ex}$ for scattering angles of mixed materials but also the behavior of functional dependencies $w_{1A1}(\varphi_j)$ and $w_{1A2}(\varphi_j)$ (see bends of curves 1 and 2; **Figure 6**), in particular, the attitude $w_{1A2}(\varphi_{2j}^{ex})/w_{1A1}(\varphi_{1j}^{ex}) \approx 0.94$.

5. Conclusions

The paper provides a brief analysis of the current state of the current direction of mathematical modeling of the process of mixing bulk components—stochastic methods for describing this technological operation. Moreover, for these purposes, the feasibility of applying the energy method proposed by Klimontovich [9, 10], due to the possibility of obtaining analytical dependences for the distribution functions of bulk components according to the selected characteristic indicator of the random process under study, takes into account the peculiarities of the state of macrosystems of mixed particles. The energy approach has been adapted to describe the mechanism of behavior of particles of loose components during their mixing in rarefied flows according to the two schemes: in combination (scheme A, neglecting collisions of different particles) and crossing (scheme B, taking into account their collisions) of rarefaction areas of mixed solid-dispersed media.

As an illustration of the work of the energy method, a generalization of the results of stochastic modeling of the formation of rarefied flows of bulk components in various working volumes of mechanical type mixers obtained on the basis of author's models that have passed verification is given. In particular, cases are considered when scattering particles of bulk materials using mixing elements fixed on rotating drums in the form of flexible bills located along a helix, according to the results of models [4, 30, 31], and brushes installed with multidirectional screw windings, according to models [2, 32–34].

Additionally, results of the stochastic model of the formation of rarefied flows of granular media when they are scattered by elastic blades mounted in tangent planes to the surface of the mixing drum are presented [13]. In particular, for this case, the analysis of the application of the described modeling method for scheme A was performed when smoothing small-scale fluctuations in the state of the macrosystems of these components due to the approximation of the unidirectional motion of different-sized particles in combined flows. It was found that at an angular rotation speed of the mixing drum of 52.36 s^{-1} , the range of variation of the spread angle for mixed bulk materials (soda ash GOST 5100-85 and natural sand GOST 8736-93) is limited by 0.758 rad excluding dispersion intervals. In particular, a pronounced discharge of particles by deformable mixing elements is observed at the initial rotation angles of the drum. Theoretical confirmation of the possible

implementation of the conditions for the effective mixing of bulk components when scattering with elastic blades on the example of obtaining a mixture of soda ash GOST 5100-85 and natural sand GOST 8736-93, reflecting the convergence of the distribution curves for the number of particles of different grades according to their scattering angle, when the following relations of values are obtained

$$w_{1A2}(\varphi_{2j}^{ex})/w_{1A1}(\varphi_{1j}^{ex}) \approx 0.94; \varphi_{2j}^{ex}/\varphi_{1j}^{ex} \approx 1.$$

The obtained analytical differential functions of the distribution of the number of particles according to the characteristic indicator of the random process under study according to the author's models [4, 34] are used to preliminarily limit the limits of variation of the design and operating parameters [31], evaluate the quality of the mixture [4, 38] and the performance of the device [39], and predict effective equipment operation modes [30]; the selection of rational ranges of parameter changes [2, 33].

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Author contributions

All authors contributed to manuscript revision, read, and approved the submitted version.


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