Stochastic Models of Solid Particles Grinding

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Abstract

Solid particle grinding is considered as a Markov process. Mathematical models of disintegration kinetics are classified on the basis of the class of Markov process that they belong to. A mathematical description of the disintegration kinetics of polydisperse particles by milling in a shock-loading grinder is proposed on the basis of the theory of Markov processes taking into account the operational conditions in the device. The proposed stochastic model calculates the particle size distribution of the material at any instant in any place in the grinder. The experimental data is in accordance with the predicted values according to the proposed model.

Keywords: Markov processes, grinding kinetics models, density of distribution.

1 Introduction

Alongside the traditional approach, based on phenomenological introduction of the mechanics of a continuous medium into a description of chemical engineering processes, in particular, milling processes, stochastic approaches, particularly those based on Markov processes, have become widely applied.

To a certain extent, these two approaches are mutually complementary. However, in many cases the detailed formal means of stochastic theory enable models of milling to be constructed more rationally [1, 2, 6, 7, 12, 13]. Stochasticity, which is an integral part of the fracture process of polydisperse material, is automatically taken into account.

Compliance with the Markov process forms the basis for modeling the particle size distribution during milling. This means that the future behavior of the system is not affected by the behavior of the system in the past [2].

It is worth noting that the methods of Markov processes have been used rather productively in theoretical analyses of many processes in chemical technology, e.g. in mechanoactivation [8], separation, classification of heterogeneous systems [9]. One of the main constructors of the statistical theory of basic processes in chemical technology was A. M. Kutepov [10, 11]. He formulated the following positive tendencies which stimulate the further development of the statistical theory of processes of chemical technology as follows:

- Interest in making active use of the methods of non-equilibrium statistical thermodynamics, the theory of casual processes and synergetic steadily amplifies.
- Constant enrichment of statistical theory by new, highly-effective mathematical means.
- Rapid development of computer technologies has enabled the creation of the automated systems for calculating and designing equipment for chemical manufacturing.
- To solve problems in simulating chemical processes it is necessary to create a bank of simple, evident mathematical models of the processes of chemical technology which are easily solved using a computer. Stochastic models of these processes obtained using fundamental methods of modern statistical theory fully satisfy these requirements.

Feller [14] reported well-arranged and inspiring review of stochastic theories in his comprehensive book.

2 Classification of grinding kinetics models

The existing variety of types of Markov processes allows the construction of stochastic models of disintegration kinetics of varying complexity that adequately reflect the specific features of the process of grinding materials in a range of milling plants.

The jump Markov process most adequately describes the impulse character of loading of solids in a shock-loading grinder. Generally, bead vibrations result in a time-continuous spectrum of actions on the material. This can be approximated by a continuous Markov process.

A classification of mathematical models of grinding kinetics, based on their relationship to a fixed class of Markov processes, is given in Table 1. This classification of models is incomplete and provisional. Nevertheless, it convincingly shows the physical conciseness of Markov models of grinding processes, and also the potential of the Markov-based methodology.

Table 1: Classification of Grinding Kinetics Models

Group No.	Markov process type	Model type	Primary disintegration mechanism	Grinder design
1	Markov chain (state-discrete and time-discrete)	Matrix	free impact	Shock mills (shock – reflective, disintegrator, etc.), roller mills
2	Markov process, state-discrete and time-continuous (transitions in casual instants)	differential – differential	constrained impact, abrasion, crushing	vibrational, magnetic-vortical, drum-type, spherical, epicyclic mills, etc.
3	jump process (time-continuous and state-continuous transition in casual instants)	integral – differential	free impact	Shock-reflective, disintegrators, hammer mills, rotor, etc.
4	diffusive process (continuous)	diffusive	abrasion	bead, sand mills, etc.
5	mixed process	integral – differential + diffusive, integral – differential + differential – differential)	abrasion + free impact, constrained impact	jet-mills: counter-current, ring, pulsating, centrifugal – counter-current, etc.

3 Stochastic models

An analysis of the milling of dispersed material in a device with a periodical action of theoretical merging, as described by the matrix model, shows that this process can be classified as a stationary Markov chain.

For this purpose, in accordance with the terminology used in the theory of Markov processes, we will introduce the concept of a vector line of probabilities of the states of the modeling system that is identical to a vector column of the size distribution of the ground material [2]

$$\begin{aligned} \pi(k+1) &= \pi(k)P, \quad k = 0, 1, 2, \ldots; \\ \pi(k)|_{k=0} &= \pi_0, \end{aligned} \tag{1}$$

or

$$\pi(k) = \pi_0 P^k, \tag{2}$$

where π_0 – a vector of initial probability distribution; $\pi(k)$ – a vector of probabilities of states in time step k; P – matrix of transition.

This is a model of periodical milling that can be developed with the help of a stationary Markov chain. However, loading particles in real conditions happens in random time instants. It is therefore necessary to describe grinding processes with the help of a discrete Markov process, bringing in what happens at casual time intervals.

It is known [4] a Markov process with continuous time and discrete states is determined by matrix A of intensities of transitions with time-constant components a_{ij} and vector π_0 of probabilities of states of the system at the initial time instant.

A mathematical description of the grinding process in this case is

$$\begin{aligned} \frac{\mathrm{d}\pi(t)}{\mathrm{d}t} &= \pi(t)A; \\ \pi(0) &= \pi_0. \end{aligned} \tag{3}$$

The solution of this equation

$$\pi(t) = \pi_0 \exp(At). \tag{4}$$

The matrix A of the transition intensities is differential, and it has a close connection with the stochastic matrix P of the transitions [4].

Let us find matrix A for a time-continuous process, for which the probabilities of conditions at moments of time $t = 0, 1, 2, \ldots$ are the same as for the time-discrete process, described by matrix P. The time of one transition of a discrete process is taken as the time unit. Comparing the solutions of equations (2), (4) at $t = k$ we can see that

$$\exp(A) = P$$

or

$$A = \ln P. \tag{5}$$

The procedures for finding the logarithmic and exponential function of a matrix are well known [5]. Expression (4) enables us to determine some of the particles of each fraction at any moment t while grinding a portion of an ideal mixture in a device.

The hydrodynamic conditions in the device obviously have an essential influence on the milling process. It should therefore be reflected in the mathematical description. In accordance with the theory of Markov processes we have introduced a theoretical analysis of the grinding process in the device of theoretical extruding of continuous action.

The equation describing the continuous process of grinding in a shock-centrifugal milling device of theoretical displacement [5] in terms of Markov processes is:

$$\frac{\partial \pi(t,x)}{\partial t} = \pi(t,x)A - v\frac{\partial \pi(t,x)}{\partial x}. \tag{6}$$

Here $\pi(t,x)$ – particle size distribution at the moment t at passage of length distance x in a theoretical extrusion device (the vector of state probabilities); v – linear speed of a stream.

Applying Laplace transformations to equation (6) twice [7], we receive an expression for the image of the vector of probabilities of states

$$\Pi(s,p) = \left(\Pi(0,p) + v\frac{\pi_0}{s}\right)(sE - A + vpE)^{-1}. \tag{7}$$

Here $L[t] = s$; $L[x] = p$;

$$\begin{aligned} L\left[\pi(t,x)\right] &= \Pi(t,p); \\ L\left[\Pi(t,p)\right] &= \Pi(s,p); \\ L\left[\pi(0,x)\right] &= \Pi(0,p), \end{aligned}$$

where $\pi(0,x)$ – vector of probabilities of states in the initial moment of time in the section specified by distance x:

$$\pi(0,x) = \begin{cases} \pi_0, & x = 0, \\ 0, & x \neq 0. \end{cases} \tag{8}$$

Here π_0 – density of distribution of probabilities of states at the initial moment, or otherwise, density of the distribution of the number of particles in the sizes at the moment $t = 0$ on an input into the device.

According to (8)

$$\Pi(0,p) = \begin{cases} \dfrac{\pi_0}{p}, & x = 0, \\ 0, & x \neq 0. \end{cases}$$

Therefore the image of the solution of equation (6) is: if $x \neq 0$, then

$$\Pi(s,p) = v\frac{\pi_0}{s}(sE - A + vpE)^{-1}; \tag{9}$$

if $x = 0$, then

$$\Pi(s,p) = \left(\frac{\pi_0}{p} + v\frac{\pi_0}{s}\right)(sE - A + vpE)^{-1}.$$

We are interested in the case when $x \neq 0$, since the density of a probability distribution at the entrance of the grinding device ($x = 0$) is known at any instant; it equals π_0.

So, having applied the inverse Laplace transform to expression (9) to a variable s, and then to a variable p, we receive the density of distribution of the probabilities of states at any point of distance x at any moment t. In other words we receive the particle size distribution in any section x at any moment t.

Note that under steady conditions $t \to \infty$ and the limiting vector of density of the probability distribution π_∞ has components dependent on the value $\dfrac{x}{v}$ and also on the initial density of the probability distribution π_0.

Setting the stationary particle size distribution π_∞ on an output of the device and having the average speed of the stream, we can define, for example, the necessary length of the device.

Using the constructed model, we can solve the inverse problem, i.e. we can find the elements of matrix A of the transition intensities. Equation (6) for vector π_∞ of the limiting probabilities of states becomes

$$\frac{\mathrm{d}\pi_\infty(x)}{\mathrm{d}x} = \pi_\infty(x)\frac{A}{v}, \qquad (0 \leq x \leq l), \tag{10}$$

where l is the total length of the grinder.

The boundary condition is

$$\pi_\infty(0) = \pi_0. \tag{11}$$

Solving equation (10) in view of boundary condition (11), we receive the density of the limiting probabilities

$$\pi_\infty(x) = \pi_0 \exp\left(A\frac{x}{v}\right), \qquad (0 \leq x \leq l).$$

Substituting for $x = l$, the elements of matrix A can be determined by solving the system of the equations constructed according to the condition

$$\pi_\infty(l) = \pi_0 \exp\left(A\frac{l}{v}\right) \tag{12}$$

and the condition of equality to zero of the sum of elements in the matrix lines.

Matrix A has following appearance

$$A = \begin{pmatrix} 0 & 0 & \dots & 0 \\ a_{21} & a_{22} & \dots & 0 \\ & & \dots & \\ a_{N1} & a_{N2} & \dots & a_{NN} \end{pmatrix},$$

where $a_{ij} = 0$, if $i < j$; $a_{11} = 0$, and

$$\begin{aligned} a_{21} + a_{22} &= 0; \\ &\dots \\ a_{N1} + a_{N2} + \ldots + a_{NN} &= 0. \end{aligned} \quad (13)$$

Thus, having received experimentally steady state distribution of particles in the sizes π_∞ on an output of the device, we can unequivocally find elements of matrix A and also elements of a matrix of transitions P. The common view of matrix P:

$$P = \begin{pmatrix} 1 & 0 & \dots & 0 \\ p_{21} & p_{22} & \dots & 0 \\ & & \dots & \\ p_{N1} & p_{N2} & \dots & p_{NN} \end{pmatrix}.$$

Considering that the elements of matrix P are formed as follows

$$P_{ij} = P_i \varphi_{ij},$$

We can find probabilities P_i of destruction of the particles of each fraction i and probabilities φ_{ij} of formation of particles of the j-*th* fraction at destruction of larger particles of the i-*th* fraction ($i = \overline{2, N}$).

Similarly, a model can be constructed for continuous milling of a dispersed material in the device of theoretical merging, modeling it by a Markov process with discrete states and in continuous time. In this case, the equation for $\pi(t)$ is [6]:

$$\frac{\mathrm{d}\pi(t)}{\mathrm{d}t} = \pi(t)A + \frac{Q}{V}\left(\pi(0) - \pi(t)\right). \quad (14)$$

Here Q – volumetric flow of dispersed material; V – operating volume of the device.

In the case of an intermediate hydrodynamic mode, the process of grinding can be simulated by means of a cell model. Thus, the process will be described by system of differential equations of type (14). The number of the equations should be equal to number of cells of the ideal mixture into which the device is broken down.

Using a set of blocks that simulate milling in a continuous action device with various hydrodynamic modes, it is possible to solve problems of modeling, optimization and constructive framing of processes combined with grinding.

The mathematical model (6, 8) of particle milling in the device of theoretical displacement of continuous action has been used to describe the process of milling in a rotor-pulse grinder. Note that the two-level shock-reflective grinder working on a single passage is close to the hydrodynamic structure of a dispersed particle stream to the device of theoretical displacement of continuous action.

If we know a vector π, describing distribution of the state probabilities, it is possible to find the density of probability distribution f, m^{-1} (or $\%/\mathrm{m}^{-1}$). This procedure is well-known in probability theory. Obviously f is identical to density of size distribution.

4 A check on the adequacy of the mathematical model

In order to obtain the experimental density of the size-particle distribution, we used the results of research on the process of grinding in a patch-centrifugal mill. The check on the adequacy of the mathematical model of grinding involves comparing the calculated density of size-particle distribution Equations (10 and 11) with the experimental density of size-particle distribution. The experiments proved that the time necessary to reach steady state conditions was a few seconds and less. As an example the results of a check on the adequacy of the mathematical model of grinding in miller are shown. Such equipment function can be described by Eqs. (6 to 13). For reasons of convenience, the calculations and the experiments used quartz of sand and benzoic acid. The linear speed of material was taken $v = 24\ \mathrm{m \cdot s^{-1}}$ in both calculations and experiments.

To obtain calculated values for the density of the size-particle distribution, it is necessary to make use of expression (12). Having determined the probabilities of particle destruction P_i and the value of the distributive functions φ_{ij}, and also the residence time of the particles $\tau = \dfrac{l}{v}$ corresponding to the regime and design parameters, we find matrix P and then matrix A ($A = \ln P$). Having substituted residence time τ, elements a_{ij} of matrices A and the coordinates of initial vector π_0 in the system of equations (12), we calculate the values for particles distribution density against particle size on an output of the device.

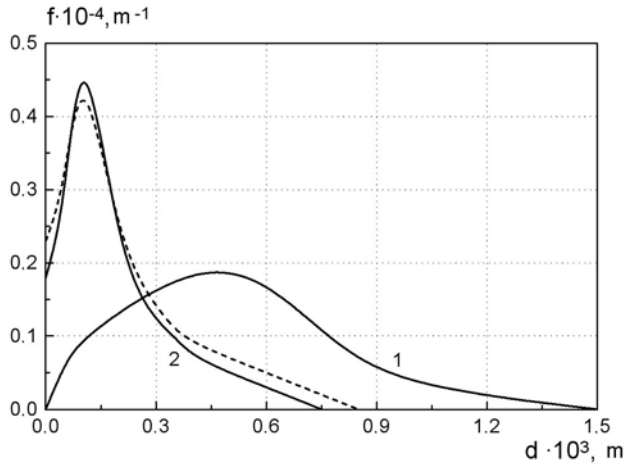

Fig. 1: Comparison of experimental density (solid lines) and calculated (dotted line) density of the distribution of quartz sand particles in sizes on an output of the device ($n = 3\,000$ rpm, $G = 100$ g/min): 1 – initial material; 2 – $t = 1$ min

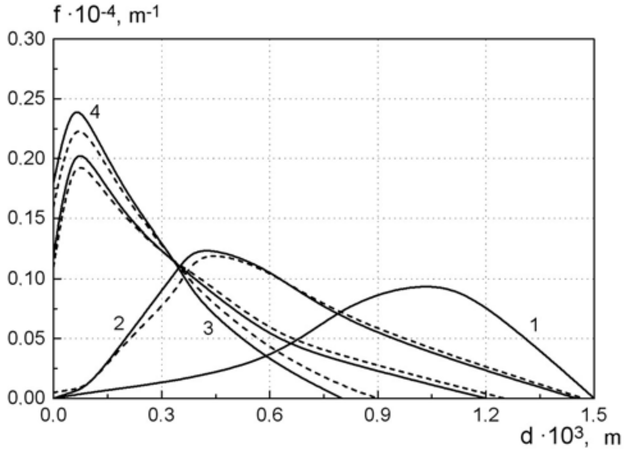

Fig. 2: Comparison of experimental (solid lines) and calculated (dotted lines) of density of distribution of benzoic acid particles in sizes on an output of the device ($G = 50$ g/min, $t = 1$ min): 1 – initial material, 2 – $n = 2\,000$ rpm, 3 – $n = 3\,000$ rpm, 4 – $n = 4\,000$ rpm

A comparison was made of the calculated and experimental particle size density distributions of the crushed material using the root-mean-square criterion of conformity [6]. Figs. 1 and 2 show the experimental and calculated particle size distribution density changes with time. Fig. 1 shows crushing of quartz sand particles, whereas Fig. 2 shows the effect of rotor rotational speed on the grinding of benzoic acid particles. Satisfactory agreement between experimental and calculated data is observed. The calculated root-mean-square criteria of the given curves do not exceed 15 %. We can conclude that the mathematical model adequately agrees with the experimental data on the crushing process.

5 Conclusion

The following conclusions can be drawn:

- Mathematical models of disintegration kinetics have been classified on the basis of their belonging to a certain class of Markov process.
- Solid particle grinding can be considered as a Markov process.
- A mathematical description of the disintegration kinetics of polydisperse particles when milled in a shock-loading grinder is proposed on the basis of the theory of Markov processes, taking into account the operating conditions in the device. The stochastic model enables the particle size distribution of a material to be calculated at any instant in any position in the grinder.
- The experimental data is in agreement with the predicted values according to the model.

Acknowledgement

This research has been executed within the framework of the analytical departmental target program Development of the Scientific Potential of the University (2009–2010). Action 2.1.2.6492 and within the framework of the agreement on cooperation between the Czech Technical University in Prague and the Ivanovo State University of Chemistry and Technology.

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Nomenclature

A matrix of intensities of transitions

a_{ij} components of matrix of transition intensities, s^{-1}

d diameter of particle, m

f density of distribution of probabilities of states which is identical to particle size distribution density, m^{-1} or $\% \cdot m^{-1}$

G mass flow of a material, $kg \cdot sec^{-1}$

i, j index of state

k time step, sec

l device length, m

L Laplacian

n rotation speed of the grinder rotor, sec^{-1}, rpm

P matrix of transition

P_i probability of particle destruction for the i-th fraction

Q volumetric flow rate of a crushed material, $m^3 \cdot sec^{-1}$

V operating volume of the grinder, m^3

v linear speed of a stream of material, $m \cdot sec^{-1}$

t time, sec

x variable, distance coordinate, m

Greek letters

φ_{ij} probability of formation of particles of the j-th fraction at destruction of larger particles of the i-th fraction

$\pi(k)$ vector of state probabilities in time step k, 1 or %

π_0 vector of initial probability distribution, m^{-1}, 1 or %

$\pi(t, x)$ particle size distribution density at the moment t at passage of distance x, m^{-1}

π_∞ stationary particle size distribution density on a device output, m^{-1}

τ residence time, sec