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Application of multi-dimensional Markov chains to model kinetics of grinding with internal classification

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Abstract

To describe the particle transport (including classification) along the main coordinate in a mill and the transition from one fraction to another (grinding), a two-dimensional Markov chain model is proposed. It allows fast calculation of all parameters of continuous grinding process in a mill for a steadystate regime as well as for a transient period. The model employs matrices of grinding and classification that are normally used for description of these processes. The model is based on standard manipulations with matrices that can be done easily using modern computer codes.

Keywords: multi-dimensional Markov chain; model kinetics; grinding; internal classification

1. Introduction

The objective of the present study is to develop a convenient mathematical tool for computational analysis of a process of continuous grinding accompanied by stochastic motion of particles in a grinding chamber. Since the process of grinding is also a stochastic process, we have a superposition of two stochastic processes that should be described. One convenient tool for this purpose that is at disposal is the theory of Markov chains.

A Markov process is a process for which, if the present is given, the future and the past are independent of each other. Sometimes they say that a Markov process "does not keep the memory on its past", or characterise it as a process without aftereffect. In terms of differential equations it means that the equations must contain derivatives with respect to time not higher than of the first order.

The theory of Markov processes was successfully applied to modelling classification and grinding (Molerus, 1967; Nepomnyastchii, 1973; Pippel and Phillipp, 1977 and many others). However, most of the first papers were devoted to mathematical aspects of the problem, and were very difficult for engineering application. The difficulties usually followed

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from presentation of a process as one with continuously distributed parameters and continuous time. In this case the governing equation of the process is a partial differential equation of parabolic type that needs a lot of far going assumptions for obtaining an analytical solution, and usually does not allow describing nonlinear effects.

A Markov chain is an important and simple example of a Markov process. It considers the sample space of a problem (the set of all possible outcomes of a random process) to be finite. A Markov chain model becomes particularly simple when it deals with presentation of time as a discrete value. In this case all the description is reduced to the matrix of transition probabilities, and matrix algebra becomes the basic tool for modelling a process.

Development of computer tools for manipulation matrices (like MATLAB, for example) has caused a new wave of interest to Markov chain models. For example, these models were successfully used for calculating residence time distribution of particles within different mills, and calculating on its basis other parameters of grinding (Tamir, 1998; Luckie and Austin, 1972; Berthiaux, 2000 and others). However, all these models deal with process development along a spatial coordinate, and transformation of particle size distribution is examined separately.

At the present study, we are going to describe two simultaneous processes: travel of a particle over the space of a grinding chamber and its transitions from one size fraction into another.

2. Basic concepts and governing equations

In order to build a simple model, let us suppose that a particle flow through a grinding chamber can be described by a one-dimensional model with a principal coordinate y. Let us also suppose that the mill length is divided into n sections and presented as n spatial perfectly mixed cells. Following this approach a particle size distribution is also to be presented as m size fractions of finite width. Thus, a particle within the mill can belong to one of the spatial sections and to one of the size fractions. The general scheme of the process presentation is shown in Fig. 1.

The $m \times n$ cells present the grinding chamber itself, and one more column of cells marked with index 'a' is added as a so-called absorbing state, which corresponds to a collector of fine ground particles. Totally the 2D array of cells has the dimension $m \times (n+1)$. The set of cells forms the sample space of the problem in question: it contains all possible outcomes of the random process of travel of a particle

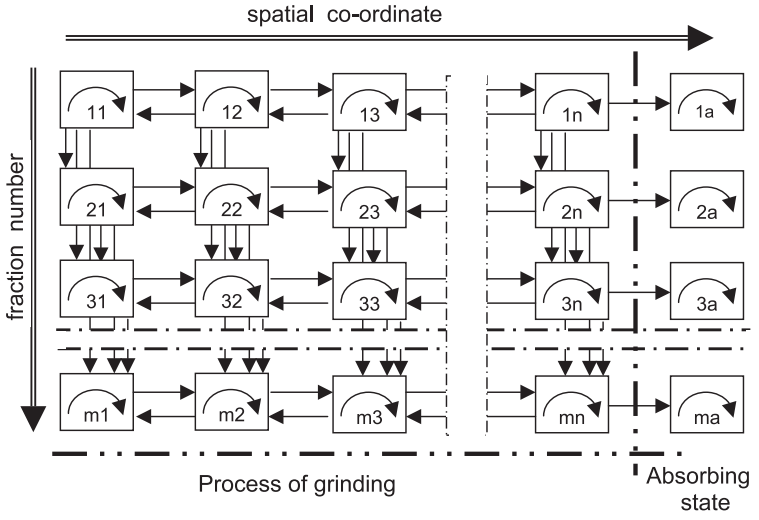

Fig. 1. A cell model of the process.

injected into the mill including its travel over size fractions.

This or that state can be occupied by a particle with a probability. A state matrix can describe the set of the probabilities for all possible outcomes

$$\mathbf{ST} = \begin{bmatrix} S_{11} & S_{12} & \dots & S_{1a} \\ S_{21} & S_{11} & \dots & S_{2a} \\ \dots & \dots & \dots & \dots \\ S_{m1} & S_{m2} & \dots & S_{ma} \end{bmatrix} \quad (1)$$

where S_{ij} is the probability that the particle occupies the cell ij. It is obvious that the sum of all these probabilities is equal to 1 because a particle has to occupy some state or other if it belongs to the process.

The objective of a model with continuous time is to predict the state matrix at a moment of time t if the matrix is given at $t=t_0$ (usually $t_0=0$). However, the model below deals with discrete moments of time $t_k=k\Delta t$, $k=1, 2,\dots$, where Δt is the duration of a transition, or the transition time. Formally time becomes an integer k, and it is connected with real time through the transition time. Thus, the objective of modelling is to predict the state matrix after k transitions if the initial state matrix is given.

A change of the state matrix after a transition takes place due to transitions of particles from one cell to another. Arrows in Fig. 1 show transitions allowed in the model. At every state a particle has the probabilities: to stay within the cell, to transit within the column to other size fraction (grinding), and to get a forward or backward transition within the row (spatial transitions). Transitions within a column are allowed to any smaller fraction ($j=1$ corresponds to the largest in size fraction, $j=m$—to the finest one). Transitions in physical space are allowed only into a neighbouring cell. It sets a limitation on the value of transition time that will be discussed below.

A particle in a cell can get a transition with a certain probability that is called the transition probability. The set of all these transition probabilities forms the matrix of transition probabilities **P** that is the basic operator of the Markov chain model. The transition matrix can be easily constructed using the following proposed algorithm:

$$\mathbf{P} = \begin{bmatrix} \mathbf{P}_{11} & \mathbf{P}_{12} & 0 & \dots & 0 & 0 \\ \mathbf{P}_{21} & \mathbf{P}_{22} & \mathbf{P}_{23} & \dots & 0 & 0 \\ 0 & \mathbf{P}_{32} & \mathbf{P}_{33} & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & \mathbf{P}_{nn} & 0 \\ 0 & 0 & 0 & \dots & \mathbf{P}_{na} & \mathbf{I} \end{bmatrix} \quad (2)$$

The matrix **P** is the block matrix consisting of $(n+1)\times(n+1)$ blocks, or matrices. Its main diagonal contains matrices of transition probabilities within columns that are of size $m\times m$, and transition matrices for forward and backward transitions within rows of cells (between columns) are placed on the diagonals neighbouring to the main one. Thus, the matrix **P** being written in numbers has the size $m(n+1)\times m(n+1)$. The column corresponding to the absorbing state is presented by the unit matrix **I**, i.e., $\mathbf{P}_{aa}=\mathbf{I}$. Every column of the matrix **P** contains all possible transition probabilities for the cell ij, and their sum is to be equal to 1.

In order to describe transformation of the state matrix **ST** from one state to another, it is to be preliminary transformed into the state column vector:

$$\mathbf{S} = [S_{11} \dots S_{m1}\, S_{12} \dots S_{m2} \dots S_{ma}]' \quad (3)$$

where $'$ means transposing a vector, or a matrix. **S** has the size $(n+1)m\times 1$.

After that, the transformation of the state vector can be described by the following formula:

$$\mathbf{S}^{k+1} = \mathbf{P}\mathbf{S}^k. \quad (4)$$

It is obvious that transition probabilities are fraction size dependent. However, the most important problem is whether they are *state dependent*, or not. Problems, in which the transition matrix **P** can be supposed to be state independent, and can be kept constant for all transitions, belong to linear problems of process modelling. In this case

$$\mathbf{S}^k = \mathbf{P}^k\mathbf{S}^0 \quad (5)$$

where $\mathbf{S}^0$ is the initial state vector obtained from the initial state matrix.

If the matrix of transition probabilities is state dependent, only Eq. (6) can be used, and the matrix is to be corrected after every transition according to a current state. Such problems belong to non-linear ones, and their solutions are normally much more time consuming. First let us concentrate on linear problems of modelling.

If the number of particles is very large, the probability of a state can be interpreted as a relative mass of particles occupying the state, i.e., belonging to the spatial section and to the size fraction. If we observe the evolution of the unit mass portion of particles injected into a mill and initially distributed as $\mathbf{S}^0$, the following process parameters can be calculated easily as:the local hold-up in the jth spatial section

$$M_j = \sum_{i=1}^{m} S_{ij}, \tag{6}$$

the total hold-up in the mill

$$M = \sum_{j=1}^{n} M_j, \tag{7}$$

the fraction size distribution in the jth spatial section

$$f_{ij} = \frac{S_{ij}}{M_j} \tag{8}$$

that also allows calculating the fraction size distribution in the ground material for $i=a$,the throughput after the jth spatial section

$$\dot{\mathbf{M}}_j = \sum_{i=1}^{m} S_{ij} p_{(i,j+1)(i,j)}. \tag{9}$$

The evolution of instantly injected mass portion of a material (a tracer) is an unsteady-state process. It is obvious that asymptotically all states will be empty excepting the absorbing ones. The distribution of the portion over the absorbing cells also gives the fraction size distribution in the ground material.

A more interesting case is the case of continuous feed to a mill. Let us suppose that the unit mass portion of the material is being injected into the mill with the distribution over the cells given by the identical state matrix $\mathbf{ST}^0$, or the state vector $\mathbf{S}^0$. The cells will be filled with material after 1, 2, …, k transitions, and the total state vector will be the sum of current ones

$$\begin{aligned}\mathbf{S}_{\Sigma}^{k} &= \mathbf{S}^0 + \mathbf{S}^1 + \mathbf{S}^2 + \ldots + \mathbf{S}^k \\ &= \left(\mathbf{I} + \mathbf{P} + \mathbf{P}^2 + \ldots + \mathbf{P}^k\right)\mathbf{S}^0.\end{aligned} \tag{10}$$

With $k \to \infty$, the absorbing cells have states $S_{ja} \to \infty$. However, for all states within the grinding chamber a steady-state finite asymptotic distribution is being formed. If we exclude from the matrix of transition probabilities and from the state vector all the elements corresponding to the absorbing cells, we get the matrix **Pm** of size $mn \times mn$, and the state vector **Sm** of size $mn \times 1$, the Eq. (12) is also valid for. As far as this equation is the matrix geometrical progression, using the formula for its sum at $k \to \infty$ we can get the asymptotic distribution as

$$\mathbf{Sm}_{\Sigma}^{\infty} = (\mathbf{Im} - \mathbf{Pm})^{-1}\mathbf{S}^0 \tag{11}$$

where **Im** is the unit matrix of the same size as **Pm**, $(\mathbf{Im}-\mathbf{Pm})^{-1}$ is the inverse of $(\mathbf{Im}-\mathbf{Pm})$. It is necessary to remind that Eqs. (12), (13) are valid only for the constant matrix of transition probabilities, i.e., for linear problems. For calculating parameters of the process within the mill there is no difference between **S** and **Sm**, and Eqs. (8)–(11) remain the same.

Thus, if the matrix **P** is known, the model allows calculating practically all parameters of the process not only for the steady state regime, but also for the transient period. However, the matrix contains too many elements, which have a clear physical sense but are very difficult to be determined. The next step of modelling is an attempt to connect these elements with well-known models of grinding and classification.

3. Decomposition of the transition matrix

In order to reduce the matrix **P** to some known matrices, let us examine some particular cases of it. First suppose that there is no grinding in the process at all. In this case all matrices $\mathbf{P}_{ii}$ become diagonal ones that means that transitions over size fractions are forbidden. Every fraction travels over the sample space along the row of cells, which corresponds to its size. Thus, we get a model for particle flow trans-

portation along the mill that can be presented by the matrix **C** that may be conditionally called as the matrix of classification:

$$\mathbf{C} = \begin{bmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} & 0 & \dots & 0 & 0 \\ \mathbf{C}_{21} & \mathbf{C}_{22} & \mathbf{C}_{23} & \dots & 0 & 0 \\ 0 & \mathbf{C}_{32} & \mathbf{C}_{33} & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & \mathbf{C}_{nn} & 0 \\ 0 & 0 & 0 & \dots & \mathbf{C}_{na} & \mathbf{I} \end{bmatrix} \quad (12)$$

where all the matrices **C** consists of are diagonal ones.

Then let us suppose that there is no particle flow along the mill that gives us independent grinding in every spatial section. In this case axial transitions are forbidden, and only transverse transitions are allowed. The matrix of grinding **G** can present this process:

$$\mathbf{G} = \begin{bmatrix} \mathbf{G}_{11} & 0 & 0 & \dots & 0 & 0 \\ 0 & \mathbf{G}_{22} & 0 & \dots & 0 & 0 \\ 0 & 0 & \mathbf{G}_{33} & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & \mathbf{G}_{nn} & 0 \\ 0 & 0 & 0 & \dots & 0 & \mathbf{I} \end{bmatrix}. \quad (13)$$

All the matrices **G** consists of are lower triangle matrices, which describe independent grinding in spatial sections.

In this case the total matrix of transition probabilities **P** can be written as

$$\mathbf{P} = \mathbf{G}\mathrm{diag}(\mathbf{C}) + \mathbf{C} - \mathrm{diag}(\mathbf{C}) \quad (14)$$

where diag(**C**) is the diagonal matrix constructed of the main diagonal of **C**.

If **C** and **G** meet the condition of normalisation in columns (the sum of elements in every column is equal to 1), **P** meets this condition automatically.

Now let us examine these matrices separately.

4. Matrix of classification

The matrix **C** controls particle flow inside the mill. In order to combine it with known models of the transportation process, let us separate a row of cells from the 2D model, and form the 1D Markov chain for any given fraction (Fig. 2).

Let us build the matrix of transition probabilities for this case on the basis of the partial differential equation of 1D diffusion with convection that was effectively used for modelling classification:

$$\frac{\partial S}{\partial t} = -V\frac{\partial S}{\partial y} + D\frac{\partial^2 S}{\partial y^2} \quad (15)$$

where V is the mean particle speed along the y-axis, D is the dispersion coefficient that characterises the stochastic component of particle motion. Both V and D are supposed to be constant with y.

Actually Eq. (17) is also related to Markov processes which are supposed to be continuous in time and space. However, if we are concentrated on discrete chains, let us take the finite difference numerical scheme of partial differential equations solution that has the form

$$S(k+1,i) = S(k,i) - v(S(k,i) - S(k,i)) + d(S(k,i+1) - 2S(k,i) + S(k,i-1)) \quad (16)$$

where $v=V\Delta t/\Delta y$, and $d=D\Delta t/\Delta y^2$ are dimensionless values, Δt is the time step of calculations, and Δy is the spatial step. The step $\Delta y=L/n$ where L is the mill length, and n is the number of the spatial sections chosen. The step Δt coincides with the duration of transition.

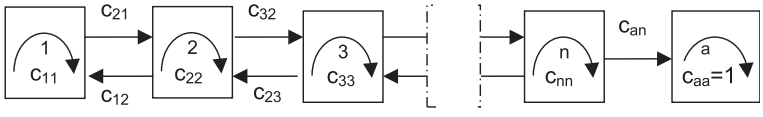

Fig. 2. Deriving the matrix of classification (1D Markov chain).

The set $S(k,i)$ can be presented as a column vector **S** of size $(n+1)\times 1$. In this case the procedure given by Eq. (18) can be presented in matrix notation

$$\mathbf{S}^{k+1} = \mathbf{C}\mathbf{S}^{k} \tag{17}$$

where the matrix of classification **C** is

$$\mathbf{C} = \begin{bmatrix} 1-v-d & d & 0 & \dots & 0 & 0 & 0 \\ v+d & 1-v-2d & d & \dots & 0 & 0 & 0 \\ 0 & v+d & 1-v-2d & \dots & \dots & \dots & \dots \\ 0 & 0 & v+d & \dots & d & 0 & 0 \\ \dots & \dots & \dots & \dots & 1-v-2d & (1-w)d & 0 \\ 0 & 0 & 0 & \dots & v+d & (1-w)(1-d) & 0 \\ 0 & 0 & 0 & \dots & 0 & w & 1 \end{bmatrix} \tag{18}$$

where the transition probability into absorbing state from the last cell w is introduced. This is an important coefficient related to the boundary condition of the third order when the flow from the last cell is proportional to the mass concentration of material in it: $\dot{M}_{an}=S_n w$. If $w=0$, the right border is presented by the absolutely reflecting screen, and an operating volume is closed from both ends; if $w=1$, it is the absolutely absorbing screen. The value of w is related to the discharge characteristics of the apparatus, and plays an important role in forming the hold-up.

As far as every element of the matrix **C** has the sense of probability, its value is to be between 0 and 1. It gives the following limitation $1-v-2d\geq 0$ that takes the following form in physical variables

$$V\Delta t/\Delta y + 2D\Delta t/\Delta y^2 \leq 1 \tag{19}$$

where $\Delta y=L/n$. Thus, if n is chosen, the value of Δt must not exceed what is required by Eq. (21)

$$\Delta t \leq \frac{1}{Vn/L + Dn^2/L^2} = \frac{L}{Vn}\,\frac{1}{1+2n\frac{D}{LV}}. \tag{20}$$

Physically this limitation means that during a transition the out-of-the-cell particle flows must not remove more material than the cell contains.

At $d=0$ (that means $D=0$) we get a particle flow without axial dispersion, i.e., a plug flow of particles. In this case, if $v=1$ (that means that the transition time is chosen as $\Delta t=\Delta y/V$), all the material transits from one cell to another during one transition. If $0<v<1$, only a part of it transits into the next spatial section.

In the simplest linear case when the matrix **C** is constant it contains three physical parameters V, D, w for every size fraction that are to be obtained from experiments or calculated from another models. This problem is beyond the objectives of the present study but it is necessary to note that there exist a lot of works devoted to different ways of the problem solution, for example, Mizonov and Ushakov (1989), Mizonov (1991), and many others.

5. Matrix of grinding

If axial transitions are forbidden (all $\mathbf{C}_{ii}=\mathbf{I}$ in **C**), every matrix $\mathbf{G}_{ii}$ in Eq. (15) describes independent grinding in the ith spatial section. Let us examine one of the matrices omitting indices. This matrix **G** is a low triangle matrix, every element of which describes a part of a fraction transited to another smaller fraction or remained within itself after a single grinding action that is related to the time of grinding Δt_0, for which the matrix was obtained. It has the following form

$$\mathbf{G} = \begin{bmatrix} g_{11} & 0 & 0 & 0 & 0 \\ g_{21} & g_{22} & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots \\ g_{m-1,1} & g_{m-1,2} & \dots & g_{m-1,m-1} & 0 \\ g_{m1} & g_{m2} & \dots & g_{m,m-1} & 1 \end{bmatrix}. \tag{21}$$

It is obvious that for the problem in question the matrix is to be restored experimentally, or obtained on the basis of a theoretical model for conditions of the batch-grinding test. The matrix **G** can be expressed through the very-often-used selection **S** and breakage **B** matrices as

$$\mathbf{G} = \mathbf{I} - \mathbf{S} - \mathbf{BS}. \tag{22}$$

However, using **S** and **B** without some special assumptions on their structure (that are normally very far from reality) does not give any advantages in comparison to the direct use of the matrix **G**. A detailed study of **G** is a very complex problem. Its elements depend on specific energies to fractions, on fraction sizes, on a hold-up, and, even more, on a fraction size distribution in the feed for grinding by compression. This all makes the problem a non-linear one. However, staying within the linear approach for grinding kinetics description it is possible to write that

$$\mathbf{G}(\Delta t) = \mathbf{G}(\Delta t_0)^{\Delta t/\Delta t_0} \tag{23}$$

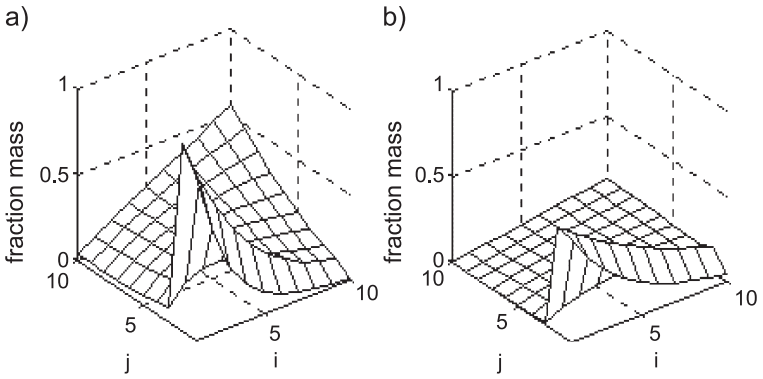

Fig. 3. Steady-state distribution of process characteristics for the plug flow model (a: V_m=0.4, w=0.4) and for the model with linear distribution of fraction speeds (b: v_m=0.8, w=0.8): d=0.

Eq. (23) allows to correspond the grinding time Δt_0 matrix **G** was obtained for, and a chosen transition time Δt from the range given by Eq. (22).

If a non-linear model of grinding, in which elements of **G** are state dependent, is supposed to be employed, the matrix **G** is to be recalculated after every transition according to the model chosen.

6. Examples of modelling

6.1. Linear Models

Examples below were calculated for constant matrices **C** and **G** that obviously gives the matrix **P** constant. All examples were done for 10 spatial sections (n=10), and for 10 size fractions (m=10). The feed material consisted of two biggest fractions in equal quantities. Calculations were done for the throughput corresponding to the unit mass per transition. For the feed rate $\dot{M}$ all elements of the state matrix are to be multiplied by $\dot{M}\,\Delta t$.

The objective of the numerical experiments is not to explain real features of grinding under these or those conditions but to demonstrate abilities of the model.

Fig. 3 shows the steady-state distributions of the process parameters for plug flow motion of fractions with identical velocities v_m, which are different for (a) and (b). The surface of the asymptotic state matrix calculated with the help of Eq. (13) can tell us practically everything about the process. The curve for i=10 practically coincides with the non-normalised fraction size distribution (these distributions are not presented on separate graphs). The summation of elements of the state vector with respect to j gives the local hold-up in the ith spatial section, the further summation with respect to i (up to n) gives the total

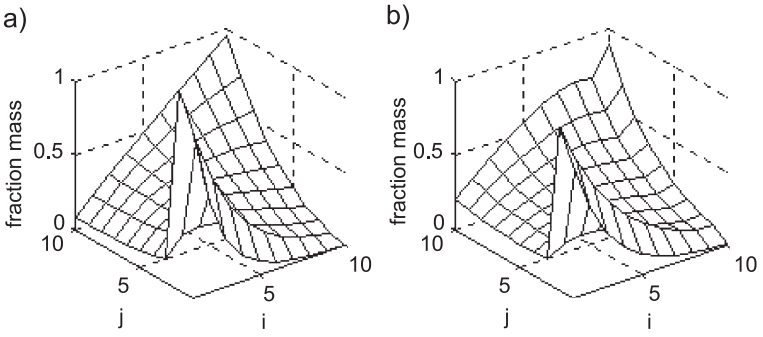

Fig. 4. Steady-state distribution of process characteristics for the plug flow model (a: v_m=0.3, w=0.3, d=0) and for the model with axial dispersion (b: v_m=0.3, w=0.3, d=0.4).

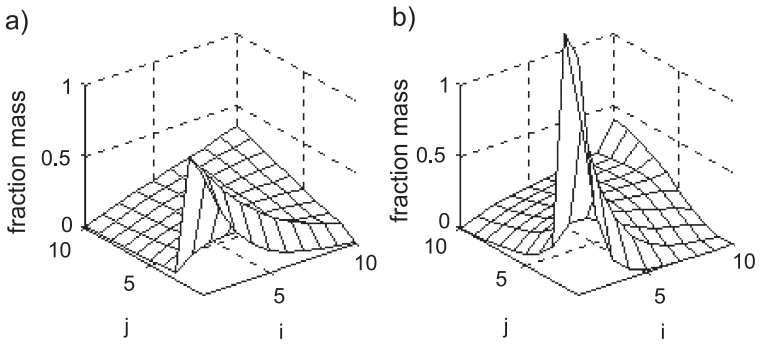

Fig. 5. Steady-state distribution of process characteristics for the plug flow model (a: v_m=0.5) and for the model with linear distribution of fraction speeds (b: v_1=0.25v_m, v_{10}=1.75v_m): w=0.5, d=0.

hold-up in the mill. All these values can be used for more precise definition of the matrices **C** and **G** in non-linear approaches.

In particular, the hold-up for the process in Fig. 3a is 24.5 units of mass, and for one in Fig. 3b is 13.2.

Fig. 4 shows the influence of the axial particle dispersion in the mill. There is no dispersion for the graph in Fig. 4a (d=0), while there is one for the graph in Fig. 4b (d=0.4). The corresponding hold-ups are equal to 33.3 and 32, respectively. The influence of the dispersion is rather small, at least for conditions chosen for comparison.

Fig. 5 shows the influence of the particle speed distribution over size fractions. Fig. 5a is related to the plug flow with identical speeds of all fractions. Fig. 5b shows the process parameters when there is also the plug flow but with different speeds of different fractions. Such distribution, for example, can take place in a ventilated drum ball mill, in which transportation of particles by air plays the most important role, and in which small particles move much faster than large ones. This distribution was taken linear with fraction size at the same mean speed v_m.

The difference in process parameters for these two cases is rather big. At first, there is the obvious difference in the fraction size distributions in the ground material. Then, despite of the fact that total hold-ups are almost equal (20 and 22, respectively), the hold-up distributions over spatial sections are very different. These distributions are shown in Fig. 6. In the case b there is much more material near the mill inlet. It can have influence on the rate of grinding, i.e., on elements of the matrix of grinding.

When dealing directly with Eq. (13) for asymptotic distribution it is necessary to take care that the condition given by Eq. (22) should be met. The point is that we can get a plausible asymptotic distribution even for an incorrect transition matrix containing, for

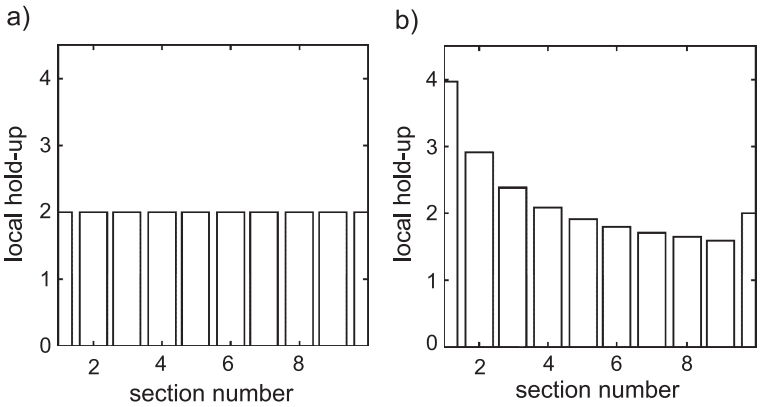

Fig. 6. Hold-up distribution over the mill for the cases shown in Fig. 5.

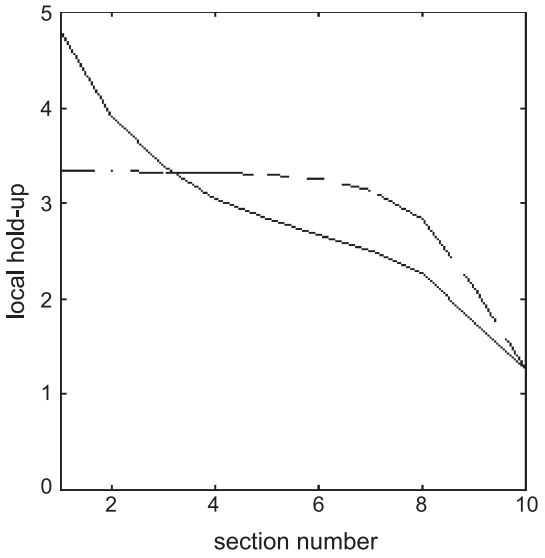

Fig. 7. Distribution of hold-up over mill lenth(- - - identical fraction velocitiess; — linear distributed): w=0.7$M_{10}^{0.5}$, d=0.2, v_m=0.3.

example, negative elements. A transient process in a mill can be observed with a computer.

6.2. An example of non-linear model

Let us examine a simple case of state dependent transition probabilities. As it was shown in Mizonov and Ushakov (1989), in a vibration mill at a certain design of the outlet system the outgoing mass flow rate is directly proportional to the square root of the material height above the outlet tube, that, in terms of the model, means that $w=\alpha M_{10}^{0.5}$ where α is the proportional coefficient. As far as the hold-up in the last section is unknown in advance iterations are required for calculation of the steady-state distribution of parameters. Depending on a form of non-linearity the iterations can converge faster or slower, and numerical experiments are required in every particular case. Fig. 7 shows examples of hold-up distribution for the model with w=0.7$M_{10}^{0.5}$. In this case 10 iterations are completely sufficient to obtain the steady state distribution. Physically the iterations are going on until the total output from the last section 10 into the absorbing cells becomes equal to 1, i.e., to the conditional feed rate to the mill. Two very different hold-up distributions meet this condition in the case of identical fraction speeds, and in the case of linearly distributed ones with fraction size speeds from 0.25v_m for the biggest fraction to 1.75v_m for the finest one.

7. Concluding remarks

The approach described above does not bring anything new in understanding physics of grinding and classification. It suggests a convenient mathematical tool for manipulating the models, which already exist, and also shows some of directions of the processes investigation. One of the main features of the approach is that it gives the universal algorithm for modelling different processes in the field, and allows to use both the models with distributed parameters and with localised ones.

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