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A Markov chain model of mixing kinetics for ternary mixture of dissimilar particulate solids

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ABSTRACT

This paper presents a simple but informative mathematical model to describe the mixing of three dissimilar components of particulate solids that have the tendency to segregate within one another. A nonlinear Markov chain model is proposed to describe the process. At each time step, the exchange of particulate solids between the cells of the chain is divided into two virtual stages. The first is pure stochastic mixing accompanied by downward segregation. Upon the completion of this stage, some of the cells appear to be overfilled with the mixture, while others appear to have a void space. The second stage is related to upward segregation. Components from the overfilled cells fill the upper cells (those with the void space) according to the proposed algorithm. The degree of non-homogeneity in the mixture (the standard deviation) is calculated at each time step, which allows the mixing kinetics to be described. The optimum mixing time is found to provide the maximum homogeneity in the ternary mixture. However, this "common" time differs from the optimum mixing times for individual components. The model is verified using a lab-scale vibration vessel, and a reasonable correlation between the calculated and experimental data is obtained.

Introduction

The mixing of powders and granular materials is of central importance for the quality and performance of a wide range of products. Bridgwater (2010, 2012) emphasized the difficulty of designing and operating the mixing process, which is largely based on judgment rather than science. The next stage of development is to build on the emerging knowledge and methods so as to clarify the basics for such designs. This will enable the process to be conducted in such a way that the mixing operation can be effectively controlled. One of the key problems in mixing dissimilar granular materials is their segregation into one another. The segregation occurs because of differences in the physical properties of the components, such as particle size, density, and shape. The action of gravity, which is always present in mixing, varies for different sorts of particles, and also leads to their segregation. With no segregation, achieving a homogeneous mixture simply involves determining an adequate mixing time. Very often, it is virtually impossible to achieve a homogeneous mixture if segregation occurs. First, the homogeneity of a mixture increases, reaches a maximum, and then decreases again. There have been a number of studies, mostly experimental, on the influence of the segregation effect on mixture quality (e.g., Jha & Puri, 2010; Jha, Gill, & Puri, 2008; Tang & Puri, 2007). However, the effect of segregation on the mixing kinetics has received less attention. In particular, it is important to estimate this effect for the mixing of multi-component dissimilar materials, when segregation becomes very complex. In a binary mixture, one component experiences downward segregation and the other component experiences upward segregation. In a ternary mixture, an intermediate component experiences both downward and upward segregation, and the evolution of its distribution becomes difficult to predict.

One way to understand the process better is to build a suitable mathematical model. Different approaches have been used to model the mixing of solids. Danckwerts (1953) and Sommer (1996) developed models based on the forced diffusion equation. These models played an important role in better understanding the mixing process and estimating the quality of mixtures. However, the analytical solutions obtained by this approach are mainly of purely academic interest. This is because of several unrealistic assump-

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Nomenclature

D	Dispersion coefficient, m^2/s
d	Probability of pure stochastic (diffusion) transition
j	Cell number counted from the top of the mixture
k	Transition number
H	Mixture height
m	Total number of cells in the chain
$\mathbf{P}$, P_{ij}	Matrix of transition probabilities and its entries
$\mathbf{S}$, S_j	State vector and its entries
S_{max}	Maximum content of mixture that a cell can contain
t	Time, s
V	Velocity of segregation, m/s
v	Probability (rate) of segregation transition

Greek symbols

σ	Standard deviation
Δt	Transition duration, s
Δx	Height of a cell, m

Indices

1	Fine fraction
2	Middle fraction
3	Coarse fraction

tions and the neglect of important physical features of the process. Kinetic theory was used by Iddir, Arastoopour, and Hrenya (2005) to model the granular mixture of components with different mechanical properties (size, density, and/or restitution coefficient), where each particle group was considered as a separate phase with different average velocity and granular energy. This model was applied to the simple shear flow of binary and ternary mixtures of particles. However, this model mostly concerned the dynamic properties of already formed mixtures rather than the kinetics of their formation. Bridgwater (2010, 2012) used discrete element methods (DEMs) to solve the main problems of mixing. However, this approach is very time consuming, which becomes a serious problem when calculating and comparing numerous process regimes and mixer configurations.

From the authors' viewpoint, one tool that is capable of solving these problems is the theory of Markov chains, which is related to the process of mixing as it describes the evolution of the state of a stochastic system. The basic idea of the Markov chain approach consists of separating the operating volume of the mixer into small but finite zones (cells) and then observing the evolution of the key component concentration in these zones at discrete moments in time, with a small but finite time step between them. This approach was used by Wang and Fan (1976) to describe the state of a mixture after passing through a static mixer. However, their work neglected the evolution of the process parameters, and did not describe the physical features of the mixing zone. In later studies by these researchers (Fan, Lai, Akao, Shinoda, & Yoshizawa, 1978; Wang & Fan, 1977), a model was developed in which transitions were only permitted to the neighboring cells.

Doucet et al. (2008)Doucet, Hudon, Bertrand, and Chaouki (2008) attempted to combine the DEM method with Markov chain theory. They computed the transition probability matrix directly using results obtained from a discrete element model. This work shows that, if accurate measurements of the state of the system are available, the associated Markov operator leads to a good estimate of the particle dynamics in the mixing system.

The general strategy of applying the theory of Markov chains to modeling different processes in powder technology was described by Berthiaux, Mizonov, and Zhukov (2005). It was demonstrated by Mizonov, Berthiaux, Arlabosse, and Djerroud (2008) that the theory can be successfully used to model heat and mass transfer between stochastically moving particulate and gas flows. The results presented below for the modeling of the kinetics of ternary mixture formation are mainly based on the approach described by Mizonov, Berthiaux, and Gatumel (2016), who modeled and optimized the mixing of two dissimilar components of particulate solids.

Theory

Suppose that it is necessary to mix three dissimilar components of particulate solids, for instance, in a vibration vessel. According to the strategy of Markov chain modeling, the total height of the mixture inside the vessel H is divided into m perfectly mixed cells of height $\Delta x = H/m$ that can exchange components after agitation. The transition of a component from a cell can occur because of pure stochastic (symmetrical) migration of particles, characterized by the transition probability d, and because of segregation, characterized by the transition probability v. The latter can be directed downward or upward depending on the component properties and their environment. The process is observed at discrete moments of time $t_k = (k-1)\Delta t$, where Δt is the time step, or transition duration, and k is the transition number, which can be interpreted as the discrete analog of time. The transition probabilities can then be calculated as follows: $d = D\Delta t/\Delta x^2$, $v = V\Delta t/\Delta x$, where D is the dispersion coefficient and V is the dimensional velocity of segregation. For the sake of determinacy, let us suppose that the only difference between the components is their size, and assign index numbers of 1–3 to the fine, middle, and coarse fractions, respectively.

At any moment of time t_k, the distribution of the volume content of the fractions over the cells of the chain is presented by the state column vectors $\mathbf{S}_1^k$, $\mathbf{S}_2^k$, and $\mathbf{S}_3^k$ of size $m \times 1$ containing elements S_{1j}^k, S_{2j}^k, and S_{3j}^k, where $j = 1, \ldots, m$ is counted from the top of the mixture.

Let us now assume that the total volume of the fractions inside each cell S_{max} remains constant with time, regardless of the composition of each fraction inside the cell. Thus, if a cell loses some of its matter during a time transition, this loss must be immediately compensated by inflows from neighboring cells. Let us assume that the value of S_{max} is equal to the conditional unit. This condition gives the following constraint

$$S_{1j}^k + S_{2j}^k + S_{3j}^k = 1, \quad j = 1, \ldots, m \tag{1}$$

The state vectors $\mathbf{S}_1^k$, $\mathbf{S}_2^k$, and $\mathbf{S}_3^k$ vary with time, i.e., from one transition to another. Their evolution can be described by the recurrent matrix equations

$$\mathbf{S}_1^{k+1} = \mathbf{P}_1^k(\mathbf{S}_1^k, \mathbf{S}_2^k, \mathbf{S}_3^k)\mathbf{S}_1^k, \tag{2}$$

$$\mathbf{S}_2^{k+1} = \mathbf{P}_2^k(\mathbf{S}_1^k, \mathbf{S}_2^k, \mathbf{S}_3^k)\mathbf{S}_2^k, \tag{3}$$

$$\mathbf{S}_3^{k+1} = \mathbf{P}_3^k(\mathbf{S}_1^k, \mathbf{S}_2^k, \mathbf{S}_3^k)\mathbf{S}_3^k, \tag{4}$$

where $\mathbf{P}_1$, $\mathbf{P}_2$, and $\mathbf{P}_3$ are matrices of the transition probabilities that control the process. It is emphasized that the matrices vary from one time transition to another and depend on the current state of the mixture. Each matrix is a tridiagonal matrix of size $m \times m$. In the general case, they have the following form

$$\mathbf{P} = \begin{bmatrix} P_{11} & P_{12} & 0 & 0 & \ldots \\ P_{21} & P_{22} & P_{23} & 0 & \ldots \\ 0 & P_{32} & P_{33} & P_{34} & \ldots \\ 0 & 0 & P_{43} & P_{44} & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{bmatrix}, \tag{5}$$

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