Powder Technology 319 (2017) 434–444

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

A non-sampling mixing index for multicomponent mixtures

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ARTICLE INFO

Article history:
Received 19 January 2017
Received in revised form 29 April 2017
Accepted 3 July 2017
Available online 05 July 2017

Keywords:
Non-sampling
Mixing index
Random mixing
Multicomponent mixtures
Powder

ABSTRACT

Uniform mixing is crucial for different types of molecules, powders, and materials in several chemical, mineral, cement, and drug companies. However, there is no effective index to evaluate the uniformity of mixing of multiple components. This study proposes a non-sampling mixing index (SMI) that is applicable to both multiple mixtures with more than two components as well as binary mixtures. The proposed mixing index estimates a mixing state by using all subdomain mixing information for all particles without requiring sampling. In the study, the index was used to predict the mixing of different types of metallic particles in a screw blender. A discrete element based numerical technique was used to determine the transient location of particles in a screw blender at different rotation rates. The effectiveness of the SMI was demonstrated by comparing it with other representative mixing indices. The effectiveness was elucidated using a model of a binary system in which two groups of particles were mixed from 0% (no mixing) to 100% (perfect mixing). The SMI indicated a linear correlation from 0 to near 1 between test mixing conditions and the mixing indices in contrast to other conventional methods that over-predicted the mixing conditions. With respect to the DEM simulation, the SMI displayed values between SMI = 0 at the initial stage and SMI = 0.9–0.94 at a fully random mixed condition for the rpm ranges corresponding to 15, 30, 45 and 60. The results also indicated that the SMI value of zero occurred at the boundaries with the exception of the bottom and that a considerably lower mixing index was obtained at boundaries as opposed to inner subdomains with respect to the fully random mixed condition ($t = 20$ s and rpm = 30).

1. Introduction

In various industries, such as food [1], drug [2], chemical [3] and cement industries [4,5], perfect mixing is essential as there are different types of particles that have different sizes and characteristics. Dough preparation in the food industry requires homogeneous mixing of flour particles (73% carbohydrate, 10% protein, and 2% fat), yeast, sugar, and salt [6]. Typically, single and twin-screw mixers are used to obtain better mixing quality [7]. In the pharmaceutical industry, small quantities of active pharmaceutical ingredients are blended with large amounts of excipients for a pharmaceutical dosage [8]. Content uniformity in drugs is very important to ensure safety and efficacy [9,10]. Inefficient blending can lead to increased variability in active components in the final dosage form, and this potentially threatens patient health [11].

In chemical and process industries, a variety of mixers including tumbler mixers, convective mixtures, high shear mixtures, hopper mixers, ribbon mixers, screw mixers and plowshare mixers are used to mix solid particles of different sizes, shapes and densities to achieve proper characteristics [12–17]. Uniform mixing of cement, soil and water is very important in the construction industry to obtain multicomponent building blocks [4,18] because the strength of a block depends on the composition of ingredients. Similarly, the performance of an asphalt pavement requires uniform mixing of multi-phase composite materials such as asphalt, cement binder, coarse and fine aggregates, and mineral fillers [19].

Computer simulations are widely used to examine the homogeneity of mixtures and to improve the design of mixers for better amalgamation. A mixing index is required to evaluate mixing conditions. Generally, the value of a mixing index should be between 0 and 1 wherein 0 implies no mixing of individual components (complete segregation) and 1 implies perfect mixing. A mixing index is used to determine optimized mixing in a specific system and it is important in identifying the design conditions of a mixer. For example, the incorrect indication of a high mixing index in a scenario involving poor mixing could lead to an incorrect decision that could result in the loss of a whole product batch. Therefore, it is very important to accurately determine the mixing index.

There are various types of mixing indices that are primarily classified into two categories. The first category is based on statistical analysis using standard deviation from spot samplings [20–23] while the other category uses all particles in a system as opposed to a few particles from samplings [24–26]. Statistical mixing indices involve critical disadvantages such as variation with sampling size and sampling conditions [27]. Specifically, it is necessary for all particles to possess a

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http://dx.doi.org/10.1016/j.powtec.2017.07.011
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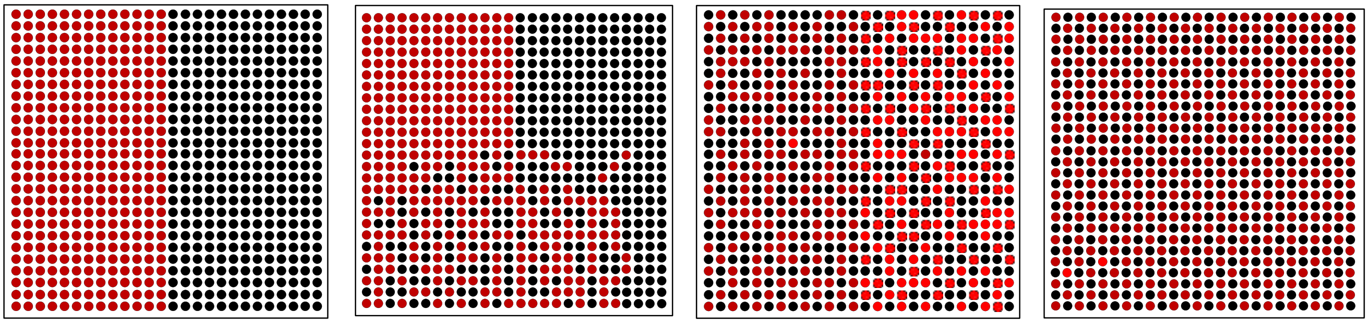

(a) (b) (c) (d)

Fig. 1. A schematic of mixing stages: (a) completely segregated, (b) partially mixed, (c) fully random mixed, and (d) perfectly mixed.

uniform size in the case of the Lacey index. The generalized mean mixing index (GMMI) uses the contribution of all particles in calculating the index [24] although the GMMI routinely over-predicts the mixing (with a mixing index higher than 1) and does not provide a single index for a mixture. Subsequently, the modified generalized mean mixing index (MGMMI) [25] was introduced to bind a mixing index between 0 and 1. However, the disadvantage of the MGMMI involves overestimating the mixing state such that it results in a value close to 1 even if mixtures are segregated.

The present study focuses on resolving existing issues in extant mixing indices by presenting a new mixing index based on subdomain analysis. The proposed method uses all particles to evaluate the mixing condition and therefore constitutes a non-sampling mixing index. The advantage of the proposed index is that it provides a linear correlation between the mixing condition of mixtures and the mixing index that is close to 0 when mixing does not occur and close to 1 when near perfect mixing occurs. In the study, the effectiveness of the index SMI was demonstrated for several model systems.

The rest of the paper is organized as follows. Section 2 discusses the advantages and disadvantages of conventional mixing indices. This is followed by introducing the mathematical basis for the proposed index. Both binary and ternary model systems are presented to demonstrate the efficacy of the proposed index when compared with other methods. This is followed by examining a mathematical model and simulation tool for a discrete element method (DEM) that is used to obtain particle mixing in a screw blender. Finally, conclusions of our study are presented.

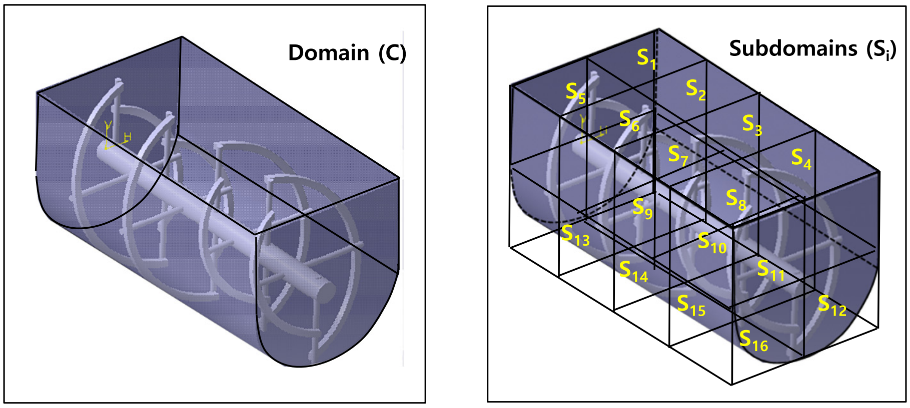
2. Conventional mixing indices

Computer simulations are widely used to design different types of mixers. These simulation tools can provide both spatial and temporal information for all particles in the computational domain. This information is readily available in a computer simulation, and thus it is desirable to obtain a method based on the locations of all particles. This section briefly discusses existing mixing indices and compares them with the proposed index.

Although perfect mixing is desirable in several processes, it is unachievable due to the tendency of particles to segregate, diffuse and display convection. Segregation occurs when a system contains particles with different sizes or densities or when selective forces are applied [28]. However, diffusion and convection prevent particles from segregating. Hence, conditions between perfect segregation and perfect mixing are obtained in actual mixing operations. Fig. 1(a)–(d) shows four different stages that may be encountered in a mixing operation. A perfectly mixed condition is rarely achieved in mixing operations. Instead, a fully random mixing state is highly likely to occur in an equilibrium mixing state owing to particle diffusion and segregation.

2.1. Mixing indices based on statistics

A variety of mixing indices were developed to essentially evaluate the quality of a mixture in field industries that require uniform mixing of two or more types of molecules with respect to their products. Most mixing indices in the literature were developed for binary mixtures and based



(a) (b)

Fig. 2. A schematic of the mixing domain. (a) Entire mixing domain C prior to sectioning (b) subdomains to estimate the mixing index. $n_w = 4$, $n_h = 2$, and $n_d = 2$. Subdomains are treated in a manner similar to three-dimensional grid elements used in the finite volume or finite element method.