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Characterizing powder mixing processes utilizing compartment models

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Abstract

Powder mixing has been the subject of substantial research due to its importance in a variety of industrial sectors, including pharmaceuticals, food, and polymer manufacturing. Although a number of different models have been proposed in the literature, most of them are either empirical or require computationally intensive calculations that make them difficult to implement for realistic systems. The aim of this paper is to develop a simplified framework, based on compartment modeling that efficiently and accurately captures the system behavior. Using the V-blender as a model system, the compartment modeling approach was used to illustrate the effects of vessel loading on mixing as well as the impact of sampling methods on the accuracy of mixing characterization.

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Keywords: Compartment modeling; Mixing models; Powders

1. Introduction

Many industrial sectors rely heavily on granular mixing to manufacture a large variety of products. In the pharmaceutical industry, it is very important to ensure homogeneity of the product. The pharmaceutical industry is one of the most representative examples, where homogeneity is very important to ensure product quality and compliance with strict regulations. Modeling can play an important role in improving mixing process design by reducing mixing time as well as manufacturing cost, and ensuring product quality. The main difficulty in modeling powder-mixing processes is that granular materials are complex substances that cannot be characterized either as liquids or solids (Jaeger and Nagel, 1992). Moreover, granular mixing can be described by multiple mixing regimes due to convection, dispersion, and shear (Lacey, 1954). Fan et al. (1970) reviewed a number of publications where powder mixing is modeled in an attempt to reduce the production cost and improve product quality. Although a complete literature survey is outside the scope of this paper, we will review the most relevant models in this introduction section.

The existing approaches used to simulate granular material mixing processes can be categorized as (1) heuristic models, (2) models based on kinetic theory, (3) particle dynamic simulations, and (4) Monte Carlo simulations (Ottino and Khakhar, 2000). Geometric arguments and ideal mixing assumptions are some common features of heuristic models. Although these models can generate satisfactory results, they are restricted to batch processes and are case dependent (Hogg et al., 1966; Thýn and Duffek, 1977). Kinetic-theory-based models are used to simulate mixtures of materials with different mechanical properties (size, density and/or restitution coefficient), where each particle group is considered as a separate phase with different average velocity and granular energy. These models typically address shear flow of binary and ternary mixtures based on the kinetic theory of hard and smooth spherical particles (Jenkins and Savage, 1983; Iddir et al., 2005; Lun et al., 1984). The main shortcoming of these models is that they focus on the microscopic interactions between particles, neglecting the effects due to convection and diffusion.

Particle dynamic simulations, which apply molecular dynamic concepts to study liquids and gases, are extensively used to simulate powder mixing (Zhou et al., 2004; Yang et al., 2003; Cleary et al., 1998). The main limitations of particle dynamic simulations are (a) the maximum number of particles required to model the system is restricted due to the computational complexity of the involved calculations, and (b) the lack of realistic particle morphology.

Monte Carlo (MC) simulations begin with an initially random configuration, which is driven to an energetically feasible

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equilibrium. One limitation of such an approach is that it cannot provide information about time-dependent characteristics, since it does not follow a realistic dynamic trajectory (Steinbach, 2005).

In order to model granular mixing processes accurately and efficiently, in this paper we explore compartment modeling. Compartment modeling has been utilized in bioprocesses to study the effects of mixing in large-scale aerated reactors (Vrábel et al., 1999) and stirred reactors (Cui et al., 1996) with satisfactory results (both qualitatively and quantitatively). Curiously, this approach has not been used to model powder mixing. The main idea of compartment modeling is to spatially discretize the system into a number of homogeneous subsections containing a fixed number of particles. Discretizing also the time domain, a number of particles are allowed to flow from each compartment to the neighboring ones at each time step. The main advantages of compartment modeling are that (a) it incorporates all associated forces responsible for particle movement within the vessel, using a flux term that can be experimentally determined and (b) it allows the simulation of a large number of particles. Although the exact particle position cannot be determined the changes in composition can be captured by including the flow of particles entering and exiting each compartment.

In this paper, the aim is to demonstrate that compartment modeling can be used to characterize powder mixing. The paper is organized as follows. Section 2 describes the central concepts of compartment modeling and how it is used here to model a V-blender, which is used as a case study. Section 3 illustrates how compartment modeling is used to elucidate the effects of initial loading on the mixing process, and determine the optimal sampling protocol including the sampling locations, the number of samples, the number of particles per sample, and sampling time. Finally Section 4 presents the main conclusions and discusses future work directions.

2. Compartment modeling

Compartment modeling has been effectively used to model the mixing of fluids in reactors to incorporate micro-mixing effects. Correa (1993) and Shah and Fox (1999) have utilized this idea to model turbulence in chemical reactors. Specifically, the fluid is represented by a large number of particles. At each time step a certain number of particles enter the reactor, while particles randomly selected from the ensemble exit the reactor at the same mass flowrate. The interactions between particles are represented by random collisions based on the mixing regime.

Compartment modeling of solid mixers is applied by spatially discretizing the system into a number of subsections that are assumed to be perfectly mixed locally (in good agreement with experimental observations) and contain a stipulated number of particles. By also discretizing the time domain, a number of particles are allowed to flow from each compartment to the neighboring ones at each time step defining the particle flux, F. The number of particles transferred account for the convective and dispersive mixing occurring throughout the vessel. Following the ideas of Fan et al. (1970), who described solid mixing as a random process, the particles selected to enter and leave each compartment are randomly selected. The change in the number of particles of species j, in compartment i, at time step k, is denoted as $\Delta\phi_{ijk}$. All of the particles in the entire mixer are represented by the sum of all the interconnected compartments (w). Thus, the change in each species j throughout all compartments at every time step must equal zero as dictated by Eq. (1):

$$\sum_{i=1}^{w}\Delta\phi_{ijk} = 0 \tag{1}$$

Compartment modeling can in principle be applied to any mixing process as long as there is enough information regarding fluxes to identify different mixing regimes, define the number of compartments needed, and model the particle flux between neighboring regions. A V-blender is considered in this paper as an illustrative case study (Fig. 1a). The V-blender rotates around the x-axis from the upright position to the downward position. The details of the process are given in Brone et al. (1998). Following the experimental observations of Brone et al. (1998), this blender can be modeled with five compartments as shown in Fig. 1b. We identify each compartment as V_1, V_2, V_3, V_4, and V_5. The particle flux between compartments V_1 and V_2 is defined as F_1, and the flux between V_2 and V_3 is defined as F_2, as illustrated in Fig. 1b.

3. Mixing analyses

3.1. Vessel composition (initial load)

Several studies show that mixing performance can be improved by perturbing the symmetry of the mixer (Cahn et

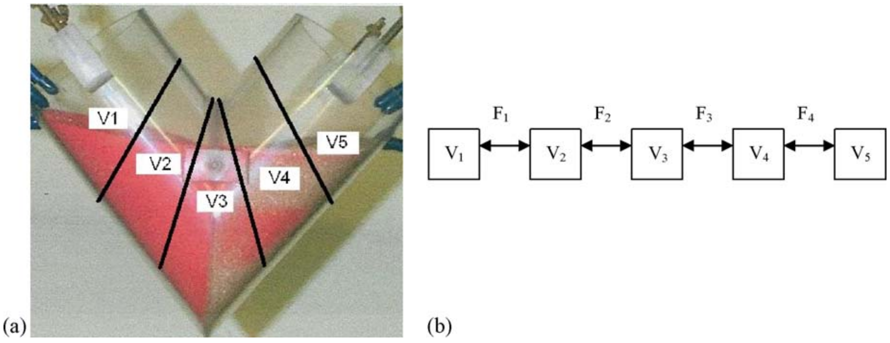

Fig. 1. (a) A discretized V-blender (b) compartment model of V-blender.

al., 1965; Chang et al., 1992; Chang et al., 1995; Brone et al., 1991). However, since this is not always a viable option for industrial scenarios, we examine the effects of initial loading. It is well known from experiments that initial loading can substantially affect the mixing process (Brone and Muzzio, 2000). Thus, the main focus of this section is to change the initial distribution of the ingredients in the vessel and examine the resulting variance profiles as a function of time. We compute the effects of initial concentration distribution on mixing time, defined as the time required to reach a homogenous state. The degree of homogenization, quantified by concentration variance, is used to characterize mixing.

The systems studied here consist of two groups of particles having different physical attributes such as chemical identity, size, and color. For the present analysis, a specific concentration is attributed to each particle group, such that the number of particles within each compartment determines the mixture concentration. Hence, in our study, one group of particles belongs to group 1 and another group of particles belong to group 2. At every time point, 100 samples from each of the five compartments are considered, each having 200 particles (the effects of sampling parameters will be discussed in the next section). In order to reflect blender symmetry, $F_1 = F_4$ and $F_2 = F_3$ (Fig. 1b). Brone et al. (1998) showed that the main barrier to mixing in a V-blender is the axial flow of particles across the vertical plane of symmetry perpendicular to the V-blender. Thus, in order to better represent geometric characteristics of this vessel, we assume that $F_2 < F_1$ and $F_3 < F_4$; i.e., F_3 and F_2 correspond to the lowest particle flux, the compartment they affect is compartment V_3, which is considered the slowest mixing region (in comparison to all the other compartments). As a case study, the particle flux is set to 1000 particles per time step between compartments V_1–V_2 and V_4–V_5 (i.e., $F_1 = F_4 = 1000$ particles per time step). The flux between V_2–V_3 and V_3–V_4 is $F_2 = F_3 = 100$ particles per time step. The resulting mixing behavior is illustrated using the variance of the system, σ^2, calculated using Eq. (2).

$$\sigma^2 = \sum \frac{(x_i - \bar{x})^2}{n - 1} \tag{2}$$

where x_i is the concentration of sample i; $\bar{x}$ is the mean of sample concentrations; and n is the number of samples.

In order to investigate the effects of initial loading, we analyze two systems with the same composition, i.e., they both contain the same total number of particles for both groups 1 and 2. As mentioned above, we are using 1 million particles in our study, and distribute evenly 200,000 particles throughout each compartment. Although the total number of particles within a vessel may be constant, the initial distribution of each type of particle may vary. For example, consider system A and system B, shown graphically in Fig. 2a and b, respectively. The numbers within the compartment represent the composition percentage of particles pertaining to group 1. For example, system A has compartment V_1 with 50% group 1 and 50% group 2, that means 100,000 particles of group 1 and 100,000 particles of group 2 initially exist within this compartment. Compartment V_2 contains 100% of group 2, which signifies 200,000 particles of group 2 initially exist within this compartment. On the other hand, case B has 200,000 particles of group 2 within vessel V_1, and 100,000 particles of group 1 and 100,000 particles of group of 2 within vessel V_2. Although both cases have the same composition (200,000 particles of group 1 and 800,000 particles of group 2), the initial particle arrangement throughout the vessel varies. Additional distributions that have the same composition are used for system C and system D, shown graphically in Fig. 2c and d. The subsequent mixing behavior of these systems is illustrated in Fig. 3, which shows the variance of the composition of samples as a function of time.

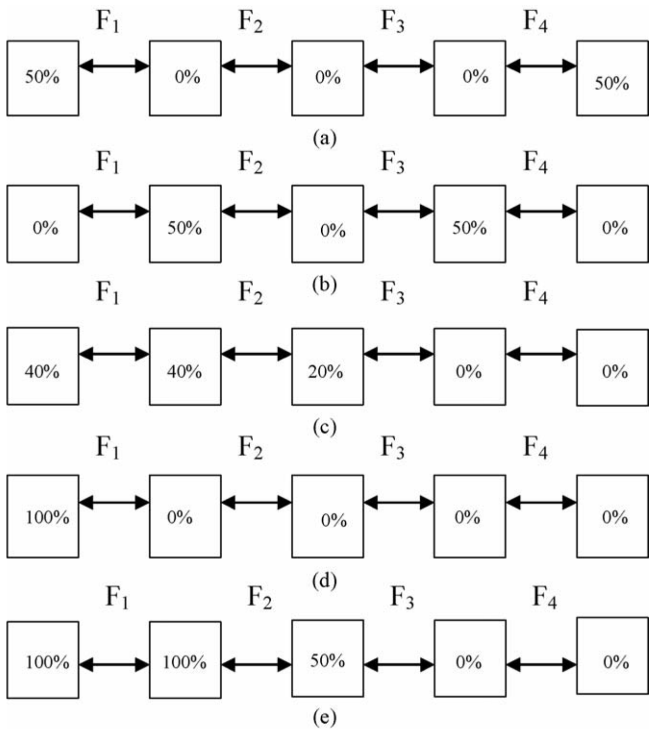

Fig. 2. The initial load distribution profiles for the following five compartment models: (a) case A, (b) case B, (c) case C, (d) case D, and (e) case E. The percentages within the compartment represent the percentage composition of particles pertaining to group 1.

As shown in Fig. 3, we significantly decrease the mixing time by varying the initial load distribution. The mixing time

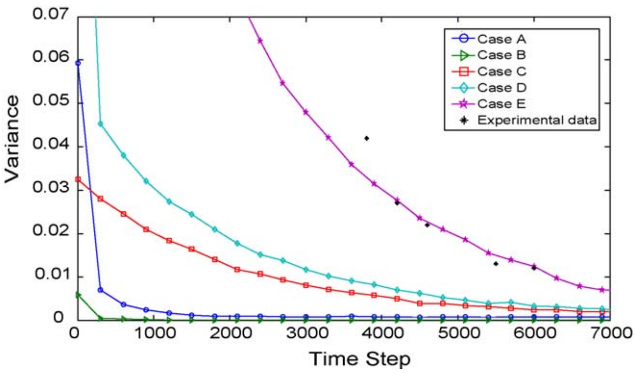

Fig. 3. Unbiased variance as a function of time steps for five cases with different loading compositions as well as experimental data from Brone et al. (1998).

Table 1
The 95% confidence interval of variance for the histogram of the variance frequencies for cases A–D for time steps [15,000, 20,000]

Case	Variance confidence interval	Δ
A	[8.98E-04, 6.99E-04]	1.99E-04
B	[1.09E-04, 4.76E-05]	6.16E-05
C	[9.12E-04, 7.08E-04]	2.03E-04
D	[9.16E-04, 7.11E-04]	2.05E-04

for system B is much lower than for system A. Thus, we conclude that system B exhibits superior mixing performance than system A. System B improves mixing because the initial load distribution of group 1, the material in the lowest concentration is closer to compartment V_3. Compartment V_3 is the slowest mixing area of the mixer, and since for system B the material distributes earlier throughout compartment V_3 than system A, and scheme B reaches equilibrium sooner.

In order to further investigate the effects of initial load distribution, two additional cases are studied, cases C and D, shown in Fig. 2c and d. Fig. 3 shows that system C results in slower mixing compared to systems A and B. This is interesting because case C has the most uniform initial distribution of particles pertaining to group 1, since it is initially dispersed throughout three compartments. However, the initial distribution is not dispersed throughout the compartments. This points to the fact that mixing time is strongly correlated to the initial load distribution. The highest mixing time of the examined cases is shown by case D, where particles pertaining to group 1 are loaded to only one area of the mixer. To further illustrate the effects of initial loading, a 95% confidence interval of variance is calculated for all cases and shown in Table 1. The results illustrate that case B has the narrowest variance confidence interval whereas case D has the widest variance confidence interval. As a result of changing the initial load distribution, the time required to reach homogeneity is reduced or increased as shown in Fig. 3.

The mixing performance of a V-blender was studied by Brone et al. (1998) given an initial load distribution. The experiment consists of two groups of particles, the materials are loaded symmetrically that is one side to the vertical plane of symmetry perpendicular to the V-blender is loaded with particles of group 1 and the other side with particles of group 2. This system is simulated by case E (Fig. 2e) and the results compared with the experimental results in Fig. 3. We load 200,000 particles of group 1 in compartments V_1 and V_2 and 100,000 particles of group 1 in compartment V_3 whereas 200,000 particles of group 2 are loaded in compartments V_4 and V_5 and 100,000 particles of group 2 in compartment V_3. The experimental results plotted in Fig. 3 from Brone et al. (1998) are obtained using one sample with 140 particles. The homogeneity of the vessel as a function of discrete time is plotted for the simulation and experimental studies. They both exhibit similar variance profiles. Variations arise due to the limited number of samples taken under experimental conditions as well as the inaccuracy that arises from sampling.

3.2. Sampling

The most common technique used to characterize a mixture is sampling. In order to properly characterize a mixing process, the sampling parameters (sampling locations, sample size, number of samples, and sampling time) must be carefully chosen to provide accurate information. In this section, compartment modeling is used to elucidate the role of sampling parameters on the characterization of mixing performance.

3.2.1. Sampling locations

An important consideration when sampling is the sampling location. As pointed out by Allen (1981), the two "golden rules" of powder sampling are that: (1) a powder is sampled only when in motion, and (2) a sample be collected uniformly from the entire process stream. Guidelines elucidate the importance of sampling uniformly throughout the mixer. However, most process analytical technology (PAT) approaches to-date sample the blender at a single location.

In this section, we examine the effects on variance of sampling at different locations within a mixing system. Initially, we examine three of the sampling schemes shown in Fig. 4 (Schemes A–C). Scheme A retrieves samples from only the middle compartment V_3, scheme B retrieves two compartments, one at each end (V_1 and V_5), and scheme C uniformly retrieves samples from each compartment (V_1 through V_5). Fig. 5 shows that using a single sampling location (Scheme A, of Fig. 4) in the center compartment severely underestimates the variance whereas two sampling locations (Scheme B, of Fig. 4) overestimates the variance. In order to monitor the accuracy among the sampling schemes we develop an optimization model where the objective is to minimize the sum of the squared difference between the variance for the uniform sampling scheme (Scheme C, of Fig. 4), σ_0, and the variance of the sampling scheme used, i, for n comparisons as shown in Eq. (3):

$$J = \sum_{i=1}^{n} \frac{(\sigma_0 - \sigma)^2}{n} \tag{3}$$

In this study, the uniform sampling scheme (Scheme C, of Fig. 4) is used as the standard for the variance distribution.

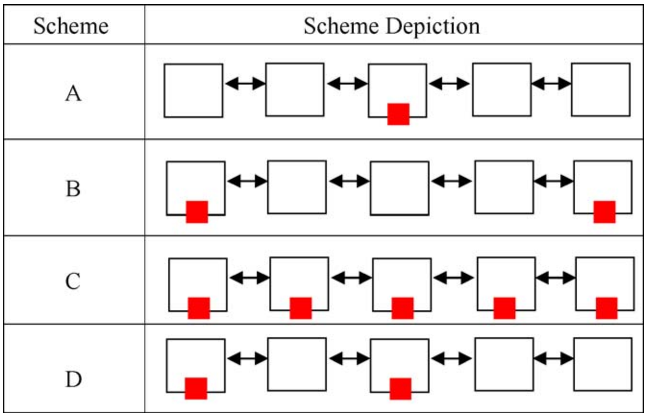

Fig. 4. Four sampling location distribution possibilities (schemes A–D).

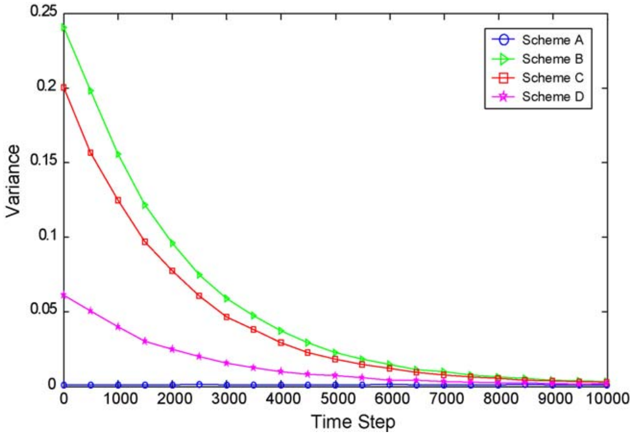

Fig. 5. Variance as a function of time steps for the four sampling possibilities (schemes A–D).

The variance difference between the standard and the sampling scheme chosen indicates the variance error. The smaller the variance error, the closer the sampling scheme represents the results of the uniform sampling scheme. The results show that case A has the largest variance error (Table 2) whereas case B has a much smaller objective function than case A, and as a result better approximates the variance distribution.

Since in most practical cases there exists a limit in the number of sampling locations that are used (i.e., 2–10), we again use a compartment model to determine the optimal sampling locations. Thus, given a constraint that only two sampling locations are allowed, the question addressed in this section is where samples should be retrieved. Considering a limiting number of sampling locations (i.e., 2), two alternatives are further investigated as depicted in Fig. 4 (Scheme B, and D). As shown in Fig. 5, these two schemes result in widely different variance estimates. Scheme B shows a higher variance than scheme D before equilibrium is reached. However, based on the objective function results (Table 2), scheme B is closer to the uniform sampling results than scheme D. If the aim is to characterize the variance of the system as accurately as possible, the goal is to minimize *J* and scheme B should be favored. Thus as illustrated by these results, sampling location is important, since distributing the same number of sampling locations differently shows dramatically diverse results. Given that there exists a large number of sampling alternatives, compartment models offer an effective way of selecting the best sampling location for a specific system.

3.2.2. Sample size

In pharmaceutical applications, the size of a single tablet is usually the scale of scrutiny where it is critical to ensure that the active ingredient is well mixed (Muzzio et al., 2004). Hence, an ideal number of particles in a sample should be equal to the number of particles in a tablet. However, this is not always possible and obtaining a microscopic sample can result in greater inaccuracy due to measurement errors, especially when using thief probes (Muzzio et al., 2003) to perform the sampling. To understand the effects of sampling methodology, the actual relationship between sample size and variance is further examined in this section.

Table 2
The objective function results for sampling location schemes A, B, and D

Scheme	*J*
A	6.2750
B	0.0349
D	0.6382

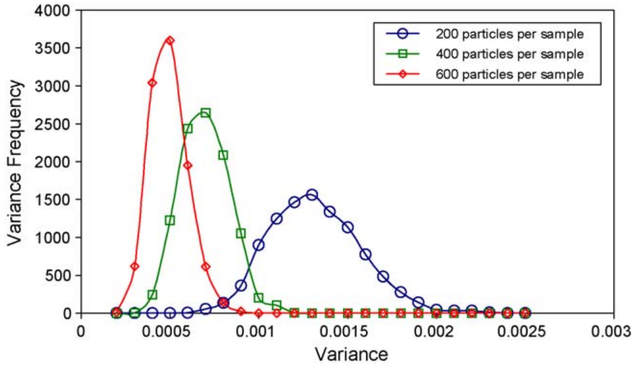

Fig. 6. Normalized variance histogram for (a) 200 particles/sample, (b) 400 particles/sample, and (c) 600 particles/sample for the time interval [15,000–20,000].

Table 3
The 95% confidence interval of variance for the variance frequency histograms of sample sizes 200, 400, and 600 particles per sample for the time interval [15,000, 20,000]

Particles per sample	Variance confidence interval	*Δ* interval
200	[1.81E-03, 7.86E-04]	1.03E-03
400	[9.37E-04, 3.96E-04]	5.41E-04
600	[6.65E-04, 2.68E-04]	3.97E-04

Consider the system in Fig. 2e (case E), we assume three different sample sizes (200, 400 and 600 particles per sample). In all cases, 50 samples are used and selected randomly at each time step and an equal number of samples are retrieved from each compartment. Although variance behavior over time is similar in all three cases (closely overlapping variance profiles), larger samples result in narrower variance distributions (Fig. 6 and Table 3). The results confirm that increasing the number of particles within each sample decreases the sample-to-sample concentration variability.

In terms of computational feasibility, using compartment models leads to very efficient calculations as shown in Table 4. The CPU times for the three cases examined are on a SUNW

Table 4
Computational results for three different sample sizes

Number of particles per sample	CPU[a] (s)	Number of iterations
200	8084	10000
400	8093	20000
600	8692	30000

The table includes the number of iterations within sampling section of the Fortran code.

[a] SUN Blade 2000.

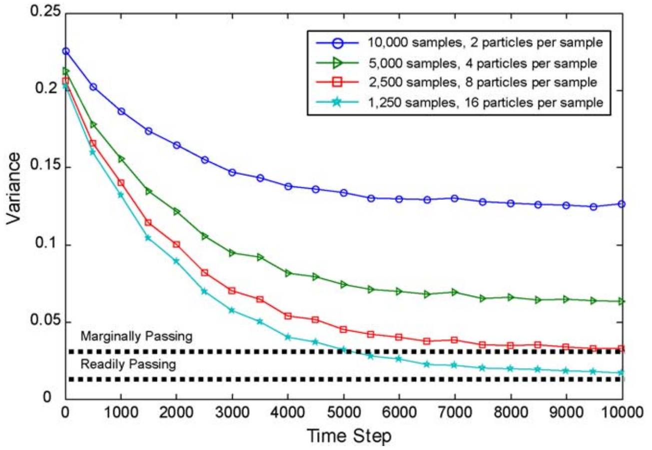

Fig. 7. Unbiased variance as a function of time steps for four sample sizes for system E.

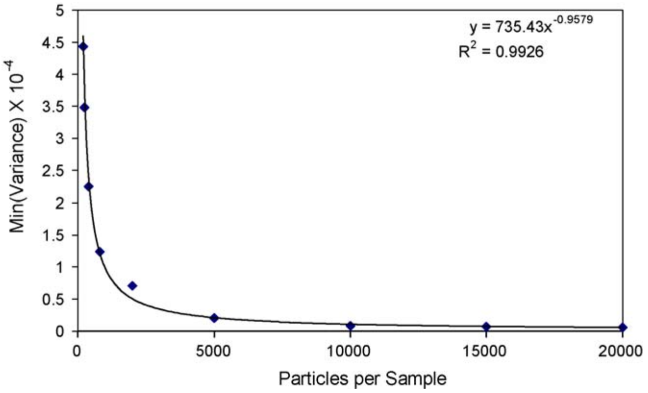

Fig. 8. Minimal variance profiles as a function of particles per sample.

SPARC Desktop (2) 900 MHz Processors 2 GB and our compartment modeling code is written in FORTRAN. When we increase the number of particles per sample from 200 to 600, the simulation takes 600 CPU s longer to run due to increased number of iterations required to achieve convergence. Although increasing the sample size increases the CPU time due to additional calculations, the simulation time remains within a feasible range in comparison to existing mixing models.

Analytical methods, such as near infrared (NIR) spectrometry, use a small number of particles in each sample (Berntsson et al., 2002), hence raising concerns about small sample sizes. To further examine the effect of sample size, we explore cases involving extreme sample sizes.

Thus, the same system is analyzed with the following four sampling sets: two particles per sample, four particles per sample, eight particles per sample, and sixteen particles per sample. The number of samples taken is adjusted to keep a constant number of particles retrieved within one time step. Fig. 7 shows a different variance profile for all the samples. As expected, sampling an identical system with more numerous but smaller samples results in a larger variance than if sampled with fewer but larger samples. As shown in Fig. 7, once the system reaches the final mixed state, the final variance value is non-zero. The higher the final variance value, the greater the variance at a mixed state. Thus, although our system is identical, each sample set displays a different final variance value. This is especially important given that in order to satisfy the existing manufacturing criteria (FDA, 2003), the relative standard deviation (R.S.D.) value should be less than 4.0% to be "readily passing" and less than 6.0% to be "marginally passing" (Many of the samples in Fig. 7 will not satisfy even the marginally passing criteria.). In order to capture the variance as a function of sample size for a given system, we analyze the minimum variance attainable for several different sample sizes of a given system. As shown in Fig. 8, in agreement with the Central Limit Theorem, the minimum variance is inversely proportional to the sample size. Consequently as illustrated with the results in this section, the variance of the system can display a large range of values depending on the sample size. Hence, setting a measurement requirement for homogeneity (such as $\sigma \leq 4$–6%) is ambiguous unless sampling parameters are defined. Thus, selection of the appropriate sample size is very important, especially for PAT methods that in practice sample very small amounts of material.

3.2.3. *Number of samples*

In the previous section, a small number of samples were considered for all the calculations. In this section, we investigate the selection of the number of samples. For the same system, we vary the number of samples used to determine the variance. The aim is to minimize the number of samples required to characterize mixing in order to reduce the adverse impact of invasive sampling (Muzzio et al., 1997). To that end, we monitor the variance evolution for three identical systems, while varying the number of samples for each system. Each case is as follows: from case 1 we take 100 samples, from case 2 we take 200, and from case 3 we take 500 samples; each sample with 200 particles. No substantial difference in variance between these three systems is observed (closely overlapping variance profiles). However, the variance frequency reveals that increasing the number of samples leads to a narrower distribution (Fig. 9 and Table 5) that visibly approaches a χ^2 (chi-square) distribution. It is also important to mention that as the number of samples increase, the average variance decreases. Variance is indirectly related to the skewness of the χ^2 distribution. As shown in Fig. 9, the skewness of the variance frequency increases as the number of samples increase.

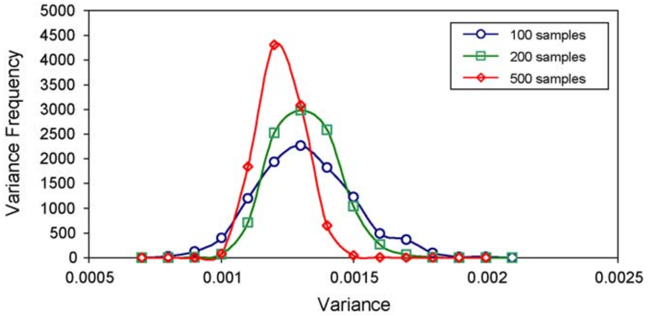

Fig. 9. Normalized variance histogram for (a) 100 samples, (b) 200 samples, and (c) 500 samples.

Table 5
The 95% confidence interval for the variance frequency histograms for 100, 200, and 500 samples at the time interval [15,000, 20,000] time steps

Number of samples	Variance confidence interval	Δ interval
100	[1.67E-03, 9.35E-04]	7.31E-04
200	[1.56E-03, 1.04E-03]	5.22E-04
500	[1.47E-03, 1.13E-03]	3.49E-04

Table 6
Compartment modeling computational results for 100, 200, and 500 samples

Number of samples	CPU[a] (s)	Number of iterations
100	8026	20000
200	8636	40000
500	9859	100000

The table includes the number of iterations within sampling section of the Fortran code.

[a] SUN Blade 2000.

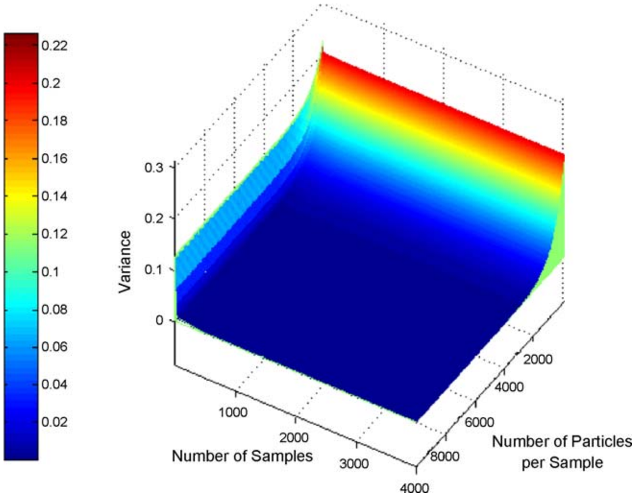

Fig. 11. Surface contour graph for two sampling variables (number of samples, number of particles per sample) as a function of variance.

Increasing the number of samples does require additional calculations, causing an increase in computational intensity. The additional samples prolong the simulation by 1800 CPU s (see results in Table 6). This may be a feasible time period considering the time length of other mixing models.

Since the number of samples is often minimized, it is important to consider the effects of a small number of samples. Thus, the following cases are considered for a constant number of particles: 5 samples of 4000 particles per sample, 10 samples of 2000 particles per sample, 20 samples of 1000 particles per sample, and 40 samples of 500 particles per sample. Although these cases showed similar variance behavior (closely overlapping variance profiles), the histograms evaluated for the time period between 15,000 and 20,000 time steps (Fig. 10) show that a small number of samples are not sufficient to represent the χ^2 distribution. A small subset of it will have a different frequency distribution than the parent group. As the samples increase, the frequency distribution more closely resembles that of the large data set. χ^2 can be used to determine what sample size will provide a reasonable approximation of the larger set. Thus, a small number of samples may not sufficiently represent the homogeneity of the system as reported by Fan et al. (1970). A contour plot is used to illustrate the relationship between the variance the number of samples, and the number of particles per samples as shown in Fig. 11. It can be noted from this plot that the smallest variance is obtained for the largest number of particles within the sample. Although increasing the number of samples also reduces the variance it is found that the number of particles per sample is the most effective factor.

The results illustrate some of the existing problems with product specifications. One problem is that setting a measurement requirement for homogeneity (such as $\sigma \leq 4$–6%) is ambiguous unless sampling parameters are defined. Secondly, the homogeneity of the mixture is not solely dependent on the mean variance, since the significance of the mean variance is dependent on the variance distribution as well as the confidence intervals. These confidence intervals are affected by the sampling set and although a homogenous mixture is present, an incorrect sampling basis will not distribute the variance as a larger sample set would.

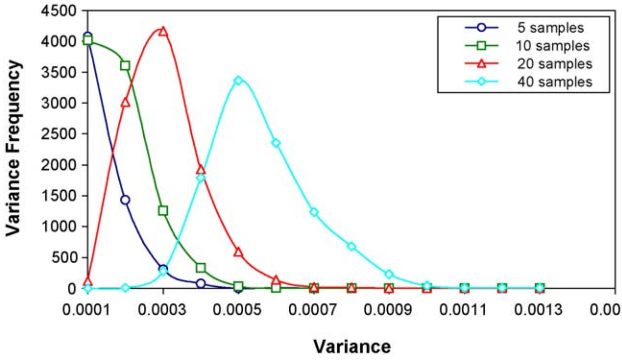

Fig. 10. Normalized variance histogram obtained for: (a) 5 samples, (b) 10 samples, (c) 20 samples, and (d) 40 samples.

3.2.4. Sampling time

Determining when the mixture has reached homogeneity is obviously important. The focus of this section is to define when homogeneity is reached in order to determine when samples should be retrieved. To investigate the effects of this parameter, we analyze the variance distributions at several time intervals. As shown in the prior variance distributions, homogenous samples (uniform datasets) distribute variance as a χ^2 distribution, given the appropriate sampling parameters. However, non-homogenous samples (non-uniform dataset) do not necessarily distribute the variance as a χ^2 distribution; this can further be read on BookRags (2006). As shown in Fig. 12, sampling at early time intervals results in variance distributions that deviate significantly from χ^2 distributions. This possess serious challenges to developing useful estimates of "goodness of fit" of measured values of σ^2.

Quantitatively, we use the χ^2 test to characterize mixing over time as proposed by Gayle et al. (1958). The χ^2 test is evaluated

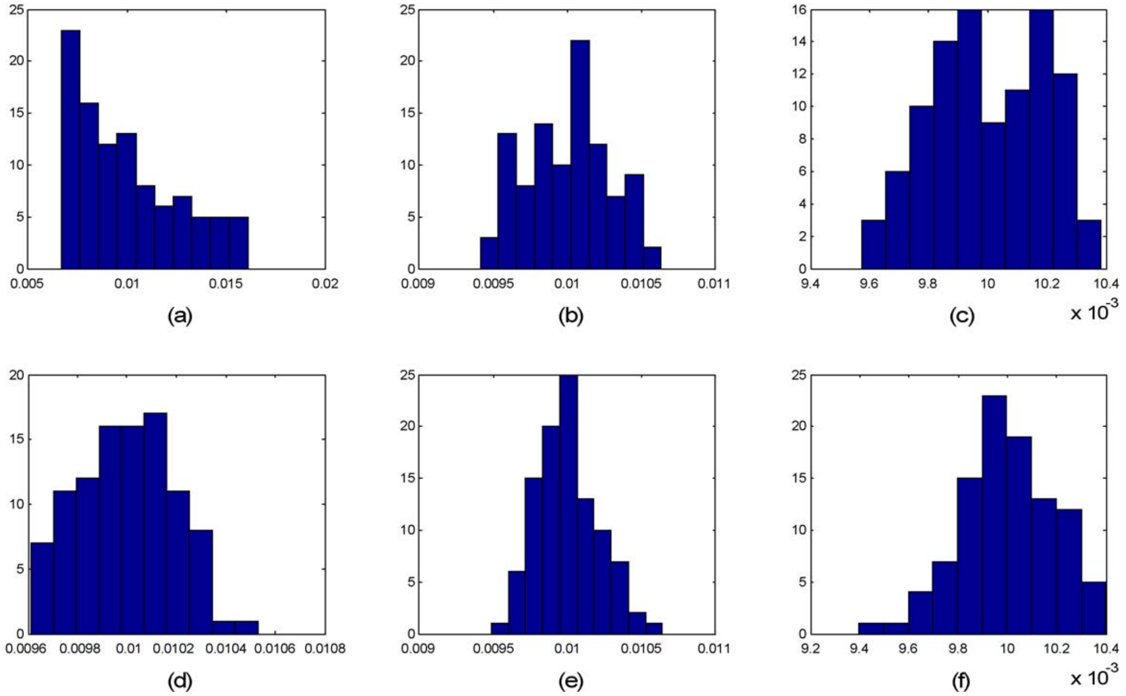

Fig. 12. Variance histogram at the following time intervals: (a) 1–100, (b) 201–300, (c) 401–500, (d) 601–700, (e) 801–900, and (f) 901–1000.

as follows:

$$\chi^2 = \sum \frac{(N_\mathrm{O} - N_\mathrm{E})^2}{N_\mathrm{E}} \tag{4}$$

where N_O, is the observed number of particles of a given physical attribute such as chemical identity, size, and color in a sample and N_E, is the expected number of particles in the mixture of the given physical attribute. When the mixture reaches a homogenous state, the χ^2 value reaches the lower limit. The lower limit is equal to the number of different components times the number of samples. In this case study, two components exist (particles pertaining to group 1 and 2) and 500 samples are taken within the mixture, so the lower limit is 1000. Table 7 illustrates the χ^2 values at different time steps. The results show χ^2 reaches the lower limit before the sample time has reached 15,000. Sampling early can be prevented by utilizing a compartment model that predicts when χ^2 has reached the lower limit.

4. Conclusions

In this paper a powder mixing process is simulated based on compartment modeling. The main advantage of the proposed approach is that the computational time is significantly reduced, allowing the simulation of a large number of particles. A V-blender is considered as a case study blender and simulated using the proposed compartment model. In terms of variance, the effects of the sample location, number of samples, particles within the sample, and sampling time are examined. It was shown that initial loading could substantially increase the required mixing time to reach a homogenous state. With respect to sampling, it was first determined that a small number of particles overestimate the variance of the system. Second, a large number of samples decrease the variance histogram width at equilibrium. Third, sampling locations can dramatically offset variance distributions. Finally, sampling early will not exhibit the variance histogram as a χ^2 distribution.

Table 7
Chi-square results at varying time steps

Sample time	Number of particles labeled with 1 at each compartment					χ^2
	1	2	3	4	5	
5000	130348	128956	100060	71271	69365	35230
10000	108896	108406	100245	91624	90829	3041
15000	102367	102870	100150	97391	97222	284
20000	101031	101099	99784	98878	99208	42
25000	100362	100024	100062	99597	99955	3.0
30000	100141	100165	100105	99810	99779	1.4

Utilizing compartment models we characterize the mixing behavior of several mixing processes under several different sampling conditions. The integration of these models to existing powder mixing processes can reduce any misrepresentation of variance profiles as well as improve mixing performance. Future work will target the development of a hybrid model between compartment model and detailed Discrete Element Method (DEM).

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