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# DEM–compartment–population balance model for particle coating in a horizontal rotating drum

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## HIGHLIGHTS

- A novel GPU-based spray algorithm is proposed.
- Area/time threshold values have a significant influence on time distributions.
- Compartment-based PB model is developed for a rotating drum.
- The compartment–PB model accurately predicts *CoV* data.
- The DEM–compartment–PB modeling approach can be much faster than DEM alone.

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## ABSTRACT

A multi-scale modeling approach combining the discrete element method (DEM), a compartment model, and a population balance (PB) has been used to predict inter-particle coating variability in a horizontal, rotating drum. In previous studies using compartment models, compartments were devised using a least squares fit to the spray zone residence time per pass (the time particles spend in the spray during a single pass through the spray zone) and the cycle time (the time between successive visits to the spray zone) distributions. In this work, the difficulties associated with measuring these time distributions are highlighted. In particular, the use of time and area thresholds used to eliminate short duration residence time correlations results in significant differences in the time distributions. A new approach that does not require area or time thresholding is used here. A compartment model consisting of a spray zone and active and passive bed zones is proposed based on the motion of the particles in a rotating drum. The parameters for the resulting coupled set of PB equations are estimated by fitting the time varying coating mass variability curve from the first few tens of seconds (35–85 s) of DEM simulation data. The long term coating mass variability (1000 s) is predicted using the PB model and compared with direct measurements from the DEM simulations. Excellent agreement was obtained between the model and DEM simulations with a relative error of less than 5% for the three cases studied. A sensitivity analysis of the parameters on the model predictions shows that the size of the active bed zone and the time scale of the exchange between the active and passive bed zones have a strong influence on the coating variability. The effective time distributions for the PB-generated spray zone residence time per pass and the cycle time were also found to be significantly different than those obtained from DEM using time or area thresholding. This new modeling approach significantly reduces the computational time required to study the particle coating process as compared to only using DEM.



## 1. Introduction

Coatings are frequently applied to particles in a number of industrial applications including those that process consumer products, food products, agrochemicals, and pharmaceuticals. Coatings are applied for a variety of reasons, such as improving a

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particle's aesthetics, changing or masking the taste or smell of a particle, improving a particle's chemical and physical stability, or changing the functionality of a particle, e.g., changing the release rate of a drug product.

Factors that are frequently considered during a coating operation include:

- Quality of the coating, e.g., surface roughness, imperfections, or particles sticking together;
- Intra-particle coating variability, i.e., the variability in coating thickness over an individual particle's surface;
- Inter-particle coating variability, i.e., the variability in coating mass from particle to particle;
- Minimum coating thickness.

Of particular interest in this work is the inter-particle coating mass variability. Some of the measurement and modeling techniques that have been used to obtain the inter-particle coating mass variability during a film coating process are reviewed in the following paragraphs.

### 1.1. Inter-particle coating variability

Inter-particle coating variability refers to the variation in coating mass that particles receive during a coating process. At any instant during a particle coating operation, the total coating mass deposited on particles will have a statistical distribution. The inter-particle coating variability, $CoV_{inter}$, is defined as the coefficient of variation of this coating mass distribution and is equal to the ratio of the standard deviation, $\sigma_{coat}$, and the mean, $\mu_{coat}$, of the total coating mass distribution,

$$CoV_{inter} = \frac{\sigma_{coat}}{\mu_{coat}}. \quad (1)$$

The smaller the $CoV_{inter}$, the better the coating uniformity. Note that it has been observed that the coating mass distribution is Gaussian at longer coating times (Mann, 1983; Denis et al., 2003; Kalbag et al., 2008).

As particles circulate in a coating pan, coating mass is deposited on the particles when they pass through the spray zone. Thus, the total coating mass deposited on the $i$th particle, $m_{coat,i}$, can be considered as a series of additions of mass to the particle,

$$m_{coat,i} = \sum_{p=1}^{P_i} m_{i,p}, \quad (2)$$

where $P_i$ is the total number of passes that the $i$th particle makes through the spray, and $m_{i,p}$ is the mass deposited on that particle during the $p$th pass. The inter-particle coating variability is, thus, a function of the distribution of the total coating mass for each particle, $m_{coat,i}$, which in turn is a function of the coating mass deposited on each particle per pass, $m_{i,p}$, and the number of passes each particle makes through the spray zone, $P_i$. Due to the inherent variability in coating equipment, particles receive different amounts of coating as they pass through the spray and different particles pass through the spray a different number of times. Thus, $m_{i,p}$ and $P_i$ can be considered random variables with associated probability density functions that need to be obtained experimentally or via computation in order to predict $CoV_{inter}$.

Treating the appearance of a particle in the spray as the occurrence of an event in a generalized Poisson process allows the coating of particles to be considered as a renewal process (Cox, 1970). It can be shown using renewal theory that at large times the distribution of the number of passes can be calculated directly from the distribution of the time between successive appearances of particles in the spray, referred to as the cycle time, $C$. Mann (1983) obtained an expression for $CoV_{inter}$ in terms of the distributions of $m_{i,p}$ and $C$, which is given by,

$$CoV_{inter} = \sqrt{\frac{\mu_C}{t}\left[\left(\frac{\sigma_m}{\mu_m}\right)^2 + \left(\frac{\sigma_C}{\mu_C}\right)^2\right]}, \quad (3)$$

where $\mu_m$ and $\sigma_m$ denote the mean and standard deviation of the distribution of coating mass deposited on a particle per pass through the coating zone, $\mu_C$ and $\sigma_C$ are the mean and standard deviation of the cycle time distribution, and $t$ is the total coating time. For a detailed derivation and discussion of Eq. (3), the reader is referred to Freireich and Li (2013). Eq. (3) shows that the inter-particle coating variability is due to the variability in two processes: the variability in cycle time and the variability in the coating mass that a particle receives per pass through the spray zone. A key assumption in the derivation of Eq. (3) is that the cycle times are independent of the spray zone residence times, i.e., the distributions are uncorrelated. Eq. (3) also shows an important trend, which is that the coating variability decreases with the square root of total coating time. In practice, however, there is a finite amount of time, depending on the coater and operating conditions, before the inverse square root of coating time trend appears in the inter-tablet coating variability. As discussed by Freireich and Li (2013), the time required to approach the asymptotic inverse square root of time dependence is related to the longest mixing time scale within the system. Therefore, systems with "dead" or passive mixing zones (as will be discussed later) exhibit an extended period where the coating variability decreases slower than the inverse square root of coating time trend.

To first order, the amount of coating that a particle receives is directly proportional to the total time it spends in the spray zone. For systems with broad particle size distributions, this assumption would be incorrect due to the particle area visible to the spray (Li et al., 2013); however, here we are mainly focused on tablet coating where the particles being coated are very uniformly sized. Thus, the mean and standard deviation in coating mass that a particle receives are proportional to the residence time per pass through the spray zone,

$$\mu_m = k\mu_T, \quad \sigma_m = k\sigma_T, \quad (4)$$

where $k$ is a proportionality constant, and $\mu_T$ and $\sigma_T$ are the mean and standard deviation of the distribution of the spray zone residence time per pass. Substituting Eq. (4) into Eq. (3) gives,

$$CoV_{inter} = \sqrt{\frac{\mu_C}{t}\left[\left(\frac{\sigma_T}{\mu_T}\right)^2 + \left(\frac{\sigma_C}{\mu_C}\right)^2\right]}. \quad (5)$$

The inter-particle coating variability can thus be determined from the distributions of cycle time and spray zone residence time per pass. For systems or models where it is assumed that the spray zone residence time per pass is independent of the bed zone residence time per pass rather than the cycle time, Freireich and Li (2013) derived the expression,

$$CoV_{inter} = \sqrt{\frac{\mu_C}{t}\left[(1-2\alpha)\left(\frac{\sigma_T}{\mu_T}\right)^2 + \left(\frac{\sigma_C}{\mu_C}\right)^2\right]}, \quad (6)$$

where $\alpha$ is the number fraction of particles in the spray zone. Although Eqs. (5) and (6) are negligibly different for realistic spray zone sizes, i.e., small $\alpha$, Eq. (6) provides a more direct comparison to compartment model approaches.

### 1.2. Residence time measurements

Clearly, the spray zone residence time and cycle time distributions play a significant role in determining the coating variability as evidenced by Eqs. (5) and (6). A number of techniques have