ABSTRACT

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Title: Modeling Granular Material Mixing and Segregation Using a Finite Element Method and Advection-Diffusion-Segregation Equation Multi-Scale Model
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Granular material blending plays an important role in many industries ranging from those that manufacture pharmaceuticals to those producing agrochemicals. The ability to create homogeneous powder blends can be critical to the final product quality. For example, insufficient blending of a pharmaceutical formulation may have serious consequences on product efficacy and safety. Unfortunately, tools for quantitatively predicting particulate blending processes are lacking. Most often, parameters that produce an acceptable degree of blending are determined empirically.

The objective of this work was to develop a validated model for predicting the magnitude and rate of granular material mixing and segregation for binary mixtures of granular material in systems of industrial interest. The model utilizes finite element method simulations to determine the bulk-level granular velocity field, which is then combined with particle-level diffusion and segregation correlations using the advection-diffusion-segregation equation.

An important factor to the success of the finite element method simulation used in the current work is the material constitutive model used to represent the granular flow behavior. In this work, the Mohr-Coulomb elastoplastic (MCEP) model was used. The MCEP model parameters were calibrated both numerically and experimentally and the procedure is described in the current work. Additionally, the particle-level diffusion and segregation correlations are important to the accurate prediction of mixing and segregation rates. The current work derived the diffusion and segregation correlations from published literatures and determined a methodology for obtaining the particle diffusion and segregation parameters.

The utility of this modelling approach is demonstrated by predicting mixing patterns in a rotating drum and Tote blender as well as segregation patterns in a rotating drum and during the discharge

of conical hoppers. Indeed, a significant advantage of the current modeling approach compared to previously published models is that arbitrary system geometries can be modeled.

The model predictions were compared with both DEM simulation and experiment results. The model is able to quantitatively predict the magnitude and rate of powder mixing and segregation in two- and three-dimensional geometries and is computationally faster than DEM simulations. Since the numerical approach does not directly model individual particles, this new modeling approach is well suited for predicting mixing and segregation in large industrial-scale systems.