Modeling Granular Mixing Processes utilizing a hybrid DEM-Compartment Modeling Approach

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Granular materials are characterized as complex substances that cannot be classified as either solids or liquids[1]. The unusual behavior of granular material is of particular importance for the formation of agglomerates in addition to unmixed regions. To model the granular flow and improve the characterization of granular materials several models have been proposed. Ottino and Khakhar[2] categorize the current mixing models as: Monte Carlo simulations, particle dynamic simulations, heuristics models, and kinetic-theory-based models. DEM simulations have been the most commonly practiced granular mixing models derived from particle dynamic simulations; however, the excessive computational power impedes the beneficial usage of the simulations to 10^5 particles in a rotating drum study as reported by Wightman et al.[3]. Monte Carlo simulations assume an isothermal system and start with an initial random configuration. The system is then driven to equilibrium by perturbations that either reduce or maintain the potential energy of the system. Heuristic models account for the mixing and segregation fluxes utilizing ordinary diffusion flux relying on physical insight. Following this approach Khakhar et al.[4] suggested that lighter particles can be considered to be immersed in an effective medium of higher density that corresponds to the average density of the mixture, whereas heavier particles can be considered to be immersed in a lower-density-effective medium. Kinetic theory based models account for the temperature gradients in the system. Hsiau and Hunt[5] results show that a temperature-induced segregation in a chute flow leads to a prediction that smaller particles migrate at the top of the layer which contradicts the prediction of Savage and Lun[6]. Our research has focused on characterizing granular mixing processes via compartment modeling that allows substantially faster results for simulations containing up to one million particles. By doing so we can determine the effect of different mixing parameters such as initial loading and determine the best sampling protocol to improve mixing characterization as specified by FDA regulations[7].

The basic idea behind compartment modeling is to spatially discretize a mixer into a finite number of compartments. A stipulated number of particles are initially loaded within the compartment where each particle is tagged with its chemical and physical identity. Time is also discretized so that at each time step a number of particles are exchanged between compartments. The particles selected to leave and enter the system are randomly chosen following the ideas of Fan et al.[8] that described solid mixing as a random process. The fluxes between compartments reflect the mixing regime within the mixer accounting for chaotic mixing and quasi-static regions.

Various mixers have been modeled using compartment modeling and compared with experimental results including a tote blender[9] and a rotating blender[3] In the present study a V-blender is examined in detail exemplifying the fact that different quantitative results can be obtained using different sampling protocols. These results illustrate that small size samples can be restrictive and not able to represent the real mixing behavior. Although increasing the size of samples result in lower variance, sampling limitations should be taken into consideration due to the invasive nature of sampling. Another source of sampling errors occurs due to the location of sensors. The addition of sensors only improves the

characterization of the mixing when the locations chosen avoid symmetrical replication. Due to limitations on the number of sensors the compartment model illustrates the difference in variance profiles obtained due to sensor location. Using the same model, we have also studied the impact of varying initial load on the mixing time. It is found that changing the locations of the load composition can decrease mixing time. In particular, by loading the limiting material in the higher mixing region results in a homogenous state much faster. In the case were material is loaded in equal proportions it is illustrated that slightly increasing the initial dispersion of the material throughout the mixer-accounting for hindered mixing regions-can significantly reduce the mixing time.

The development of mixing models to efficiently simulate the behavior of granular material in a complex region is subject of continuous research. Bertrand et al.[10] presented a review of the advances occurring in the field of granular materials and DEM models. The addition of a moving impeller within the granular mixing process has resulted in additional modeling strategies to account for this moving boundary. One strategy is based on discretization of the boundary surfaces by means of a finite-element mesh that can be generated with a mesh generator known as multi-wall method established by Kremmer and Favier[11]. Another approach is developed by overlapping a series of particles replicating a boundary domain. This boundary consists of an assemblage of particles with physical properties that mimic the interaction between a wall and particle and is used by Cleary et al.[12] for the case of a rotating drum. The increase in computational intensity occurring in the system within this area is unavoidable due to the physical complexity of an impeller. Currently some DEM case studies show that within a sufficient fill level the physical actions of the impeller no longer affect the vessel contents within certain sections.

Taking advantage of these findings we propose a hybrid model that utilizes DEM and a stochastic compartment model in order to properly model the granular particle behavior within a mixer enclosing an impeller. A similar approach is proposed by McCarthy and Ottino [13] that combined particle dynamics and geometric insight to form a hybrid technique for a tumbler operating in the avalanching regime and a continuous flowing tumbler. In the proposed approach DEM simulations are used to determine the interactions between the impeller and particle collisions. Utilizing moving boundary surfaces within a vertical mixer we monitor the impact of the impeller in the system. The particle trajectories are solved using Newton's equation of motion. Each particle may interact with its neighbors or with the boundary at contact points through normal and tangential forces. Walton and Braun's partially latching spring model[14] is utilized in these studies. DEM discretizes the mixer spatially to account for potential particle or boundary collision partners within their grids. DEM is used at the region around the impeller and accounts for the oscillatory normal forces occurring throughout impeller rotations, accounting for the time dependent particle fluxes occurring within the impeller grid region. Areas that are not directly experiencing the moving impeller rotation are modeled using a compartment model that describes particle movements utilizing the input from particle circulation. In this way, we can monitor the particles that are initially within the quasi-static regime and approach the inertial area and vice versa. At every time step, a number of particles are interchanged between DEM region and compartment modeled regions. These particles are found at the DEM and compartment model interface. In the case of a vertical stirred mixer we capture the impeller area using DEM and the surrounding area is modeled using compartments. In this way a detailed description of the mixer can be achieved reducing the computational complexity of the mixing simulation substantially.

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