ABSTRACT

Freireich, Ben J. Ph.D., Purdue University, December 2010. A Compartmental Approach to Studying Particle Motion in Mixer/Coaters Using Discrete Element Modeling . Major Professor: Carl R. Wassgren, School of Mechanical Engineering.

Systems of particles can be modeled in a number of ways. The discrete element method (DEM) is among the most detailed of all possible approaches. When using DEM, the trajectory of each and every particle is computed. Naturally, this comes at a high computational cost. At a more abstract, vessel scale level, population balance (PB) modeling is also used. In this approach a system of partial differential equations is written (similar to the conservation equations of mass, momentum, and energy) which describes the evolution of the distribution of particle properties (*e.g.*, size, composition, and age). Unfortunately PB cannot directly account for the motion of material in a vessel in a computationally efficient manner.

In this work, a novel multi-scale modeling approach is presented in which DEM and PB models are combined via a compartment model (CM) to account for flow heterogeneity in a particle mixer-coater. Using this approach, the mixer is decomposed into bed and spray regions, and particle trajectories taken from the DEM model are used to generate an intermediate sub-CM that matches the residence time distributions of particles in these regions. A system of PB models is then generated from the CM. The CM presents a simplified, but still accurate description of the particle residence times in the regions of the mixer. A case study of a simple top spray coating system shows the method is 80% faster than using DEM alone with 13% of the error of using PB alone. Approaches to estimating the minimum DEM simulation time are also presented. Parametric studies are performed which demonstrate that as operating parameters of the mixer are varied, the CM structure remains and only the CM parameters change. This fact allows generation of a single CM structure for

a given system. The method is applied to three mixer geometries: a dual-axis paddle mixer, a horizontal axis rotating drum, and a vertical axis mixer.

The approach is limited to systems in which the residence time in a region is statistically independent of the residence time in any other region. Also, a region's residence time distribution must be able to be modeled in terms of a network of ideal compartments. The mixer flow must also have reached a steady state so that each region's residence time distributions does not vary with time. Within these constraints, the multi-scale modeling approach developed in this thesis is capable of drastically reducing computational time and increasing total process understand via the reduction of a full DEM simulation to a simple CM.