ABSTRACT

Sinha, Tuhin Ph.D., Purdue University, December 2011. Investigation of Compaction, Young's Modulus and Tensile Strength of Binary Powder Mixtures using the Multi-Particle Finite Element Method (MPFEM). Major Professor: Carl R. Wassgren Jr., School of Mechanical Engineering.

The compaction of particulate systems can be simulated using phenomenological elasto-plastic continuum models adopted from soil mechanics. These constitutive models, like the Drucker-Prager Cap (DPC) model, have been successfully implemented in a finite element method (FEM) framework to model compaction unit–operations in various powder processing industries such as powder metallurgy, ceramics and pharmaceuticals. The constitutive model parameters for these phenomenological models are determined by simple, but tedious experiments. So far, this method has been effectively applied to model single species of powders. However, for scenarios involving a mixture/blend of powders, such as practical pharmaceutical formulations, implementation of the above modeling method requires repeated calibration experiments for every mixture. Thus, it would be advantageous to have a rule of mixtures that could predict the model parameters of blends from single component values.

The objective of the current research is to take the first step towards developing feasible mixing rules for binary/two–component powder mixtures. Multi-particle finite element method (MPFEM) methodology is used to analyze binary mixtures by performing probing studies on a small, representative volume element of particles. The models developed using this approach are used to explain the reason behind experimentally observed property trends in binary mixtures. In the current work three specific scenarios are investigated using the MPFEM approach: compaction behavior of binary mixtures, and the resulting compact's elastic modulus and tensile strength.

The compaction analyses examine the role of particle material property and particle size differences on the overall compaction response of binary blends. The results of these studies demonstrate that differences in particle material properties influences the mean yield pressure during compaction; however, differences in particle size alone does not have any considerable effect on the compaction response of blends with varying volume fractions of coarse and fine particles.

The elastic modulus of binary mixtures is influenced by both, particle material property and particle size variations in blends. For all the analyses, the elastic modulus varies non–linearly with the mixture constituent fraction and cannot be predicted by using a simple, linear relationship between the elastic modulus of individual components and their blend volume fractions. Further, the analyses results also reveal that the elastic modulus of mixtures is always bounded by the modulus of individual components.

The tensile strength analyses show that the overall strength variations in a mixture is dependent on the dominance of adhesive/cohesive inter–particle bonds between the constituent materials. In addition to that, the tensile strength of a particulate system is dependent on the inter–particle bonding area and the MPFEM results highlight that the tensile strength of a mixture increases with increasing the inter–particle bonding area. It is also observed that the strength of a binary mixture increases with reducing the particle size, since it increase the net bonding area in the resulting blend.

These studies provide a deeper understanding of the relationship between microscopic and macroscopic properties of particulate compacts and help in comprehending the effects of micro–structure manipulations on the macroscopic response of binary mixtures.