IFPRI Project Abstract

Model Assisted Design of Granular Products: Linking Process and Product Models for Wet Granulation

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Project Objective:

The objective of this project is to develop multi-dimensional process models of binder agglomeration that have as their output the appropriate particle properties (likely distributed) that are linked to associated product models to predict product performance. The project scope is constrained to high-shear and/or fluid bed granulation, however the choice of formulation(s) and modeling approach(es) are open.

Approach:

The aim of this research project is to develop a modeling framework for product performance driven process design which is deployable to industry, and demonstrate the potential of this strategy. This will involve the development and linking of population balance models for wet granulation with a mechanistically-based product model.

Recent Results:

In previous years, a computational model for the prediction of swelling driven dispersion and disintegration of granular products was developed. This model coupled a "single granule mode" for granule swelling with a population balance model (PBM) to give the evolving particle size distribution. Efforts in the past year have focused on final model troubleshooting and implementation in gPROMS, global sensitivity analysis and model validation and parameter estimation.

A method for experimentally evaluating bulk granule dispersion and disintegration using FBRM was developed, and experiments were conducted to validate and parameterize the PBM. It was found that there was good agreement between experiment and model for a formulation containing microcrystalline cellulose, however predictions for the formulation containing dibasic calcium phosphate were somewhat less accurate. This inaccuracy is most likely due to key assumptions on agglomerate fragment size distributions made in the model, which can be addressed in further model iterations.

Next Steps:

The model for granule dispersion and disintegration is now largely complete and validated. Although further improvements are possible, our primary focus will be 1) Parameterization of our PBM for High Shear Wet Granulation, 2) Linking the process model with the disintegration model, and 3) Applying inverse problem-solving techniques to demonstrate model driven design of granulation.