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, and advanced data driven techniques to solve the inverse problem.

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. These models were parameterized using experimental data generated at the University of Sheffield and the University of Strathclyde.

In the past year, focus has been placed on developing the methodology to solve the inverse problem, i.e. for a given desired disintegration performance, predict the required processing parameters and material properties. A framework for achieving this has been proposed, incorporating the previously developed mechanistic models, Generative AI, Machine Learning Techniques, and Bayesian Optimization. The inverse method has been implemented into a User Interface and preliminary results are promising.

Next Steps:

Using the recently developed and implemented modelling framework, we will return to the mechanistic model for granule disintegration, with a focus on generating larger data sets for data-driven model training. Alternative inverse modeling approaches will be evaluated, and small quantities of good quality experimental data will be generated for model validation. The approach will be extended to include the wet granulation process model, in addition to the currently implemented disintegration model.