

Feasibility/Collaboration Proposal: Model calibration as a Tool for Material Characterisation

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Introduction and Background

Constructing and solving complex mathematical or computational models for powder processes invariably requires a process of parameter estimation and calibration. In developing mechanistic models, we endeavour to reflect realistic physical and chemical interactions where possible, including fundamental properties of powders and liquids as model parameters such as particle size distributions, particle and granule porosity, liquid viscosities, solid-liquid contact angle, surface tension, etc. Despite the inclusion of mechanistic mathematical descriptions and measurable properties, most models must still include fitting parameters which may have no direct physical meaning. These fitting parameters are used to calibrate the model, often to account for un-represented interactions, simplifications due to model assumptions or non-ideal behavior.

In most instances, efforts are made to measure material and system properties where possible, and use these measurement as model inputs. However, with increasing ability to reliably model both powder process and formulated product performance, there is **an excellent opportunity to investigate the ability of models to *predict* material properties, using the parameter estimation process. If successful, this procedure may turn computational models into characterization tools.**

In the IFPRI project *Model Assisted Design of Granular Products*, we are investigating the feasibility of linking process models with product performance models to enable solving of the inverse problem, i.e. predicting the required process parameters to achieve desired product performance. As part of this work, we have developed a new model to predict the swelling driven disintegration/dispersion of granular products in liquids. This model consists of two coupled sub-models: a single granule model in which swelling and resultant internal stress evolution is considered, coupled with a population balance model which accounts for the change in a population of granules with time due to breakage and swelling. We propose to investigate whether it is possible to use our model as a material characterization tool.

Proposal Aims and Objectives

The aim of this feasibility project is to test the hypothesis:

Can the process of parameter estimation be used to characterize particle and/or other material properties?

The process of parameter estimation and model calibration itself involves the use of inverse problem solving techniques; we know the desired “result”, and are trying to establish the values for the parameters which give the best approximations within the experimental space provided. This feasibility project presents an opportunity to deliberately use the parameter estimation process to “measure” (i.e. predict using inverse methods) particle and material characteristics. These predicted characteristics, including properties such as constituent particle size or granule porosity which are routinely required for several aspects of particle process design and modelling, would then be compared with carefully experimentally measured properties.

The newly developed coupled model for granule disintegration poses interesting challenges and opportunities for verification, validation and calibration. The entire coupled model can be validated

simply using measured evolving particle size distributions, however calibration at only this scale without separately calibrating the single granule model may result in increased uncertainty in the parameter estimation. By collaborating with Daniel Markl at the University of Strathclyde, we will be able to use new, cutting edge techniques to additionally validate the single granule model, and to investigate the ability of the model to predict material and powder properties. In particular, Dr Markl has recently installed an Optical Coherence Tomography (OCT) apparatus for the in-situ study of tablet and granule swelling, disintegration and dissolution. This equipment, and the existing Terahertz Spectroscopy tool at the University of Strathclyde, have unique potential to examine liquid penetration and particle swelling in tablets and granules.

A feasibility/collaboration grant is requested to enable this study, and to fund collaboration between Daniel Markl at the University of Strathclyde and Rachel Smith at the University of Sheffield. This collaboration grant would fulfil four distinct objectives:

- 1) Using this model as a case study, interrogate the ability of the model to predict material and particle properties, by intentionally and systematically varying those properties which are estimated through the model calibration process, and those which are used as model inputs.
- 2) Assess the sensitivity of the model to particle and material property measurements, and critique the value of accurate characterisation for this model.
- 3) Based on the results of this case study, provide guidance on future work for model predicted property characterisation for particulate processes and products.
- 4) Provide an opportunity to validate elements of the single granule model, improving model confidence for the existing IFPRI project.

The requested funding would be primarily used to enable researcher travel and subsistence while conducting substantial experiments at the University of Strathclyde.