

Precision powder feeding: Theoretical understanding and predictive modeling to link material properties to the performance of twin screw feeders

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Scope

This effort addresses the International Fine Particle Research Institute (IFPRI) Research Grant Opportunity: Modeling Precision Feeders. The proposed research project aims at: (i) developing and implementing a predictive continuum model for predicting twin screw feeder performance and (ii) validating the model with results from an experimental characterization campaign conducted using a powder and a screw geometry relevant to IFPRI members.

Background

Powder feeding is critical in a wide array of manufacturing processes since the feeding step sets the mass flow rate and ratio of a formulation's components. If critical formulation components cannot be fed in a controlled manner, then the resulting product may have unacceptable quality. Unfortunately, many powders have poor flow properties, including being highly compressible and cohesive. Models that can provide guidance on how to better design and operate a screw feeder for poorly flowing, or "difficult", powders is highly desirable.

A number of screw feeder and screw conveyor models have been previously published, with many of these previous works focused on "well-behaved" materials. These previous works have included empirical (Rehkugler and Boyd, 1962; Das and Grace, 2011; Sander and Schonert 1999), analytical (Darnell and Mol, 1956; Tadmor and Broyer, 1972, Lovegrove and Williams, 1973; Hyun et al., 1997; Yu and Arnold, 1997; Das and Grace, 2008; Patterson, 2014), and computational (Hong et al., 2007; Moysey and Thompson, 2008; Owen and Clearly, 2009; Kretz et al., 2016; Mazor et al., 2017) studies to predict flow patterns, stresses, mass flow rate, and screw torque/power, with a focus on non-cohesive materials and single-flighted screws.

Empirical models rely extensively on experimentation. Such models are essentially curve fits to considerable experimental data. As such, their generalizability to feeder designs and materials not used to generate the data is questionable. In addition, empirical models provide little fundamental understanding concerning a process. The analytical models on screw feeding provide excellent fundamental insight, but must rely on modeling simplifications and assumptions in order to be manageable for analysis. These simplifications significantly limit their use for practical implementation, e.g., the current published analytical models are for incompressible, cohesionless materials in simple screw geometries. The state-of-the-art computational models utilize the discrete element method (DEM), which tracks the movement of individual powder particles. These models have good generalizability, but the DEM method is limited by the number of particles that can be tracked computationally. As a result, the models assume particles are much larger than in reality, e.g., particle diameters on the order of millimeters as opposed to microns, with simplified properties, e.g., particles are assumed to be

spherical. Furthermore, the particle properties used in DEM models are challenging to measure, making their quantitative predictions questionable.

This proposal describes a continuum computational model for predicting screw feeder flow dynamics. This approach is generalizable, provides fundamental insight, and avoids the limitations and difficulties found with the DEM approach. In addition, the PIs have previous experience applying similar continuum models to tableting (Sinha et al., 2010a, 2010b; Swaminathan et al., 2016), roll compaction (Muliadi et al., 2012a, 2012b; Liu and Wassgren, 2016), and blending and segregation (Liu et al., 2018a, 2018b, 2018c) powder systems with excellent quantitative success.

Proposed Objectives

This three year project has the following objectives that work toward the goal of developing, implementing, and validating a predictive continuum model for predicting the feeding dynamics of powders in a screw feeder and, thus, understanding equipment performance.

1. Produce a literature survey document summarizing published theoretical and empirical models for predicting screw feeder performance.
2. In collaboration with IFPRI, obtain a computer aided drawing (CAD) model of the screw, barrel, and hopper geometry of a “target” twin screw feeder.
3. In collaboration with IFPRI, identify a powder to be used in model and experimental testing. The powder should be safe for handling in a university laboratory environment.
4. Obtain modified Drucker Prager Cap (mDPC) elasto-plastic constitutive model properties of the powder identified in Objective 3. These properties will be measured at the Particle, Powder, and Compact Characterization Laboratory located at Purdue University, or obtained from the literature. The mDPC properties include the powder’s elastic modulus, Poisson’s ratio, cohesion, internal friction angle, cap eccentricity, and hydrostatic yield stress. These properties will be made for the range of solid fractions anticipated in the screw feeder. The model will not account for interstitial fluid effects or strain-rate dependence.
5. Develop a continuum model using the finite element method (FEM) with an mDPC material model to predict material flow dynamics, screw torque, powder bulk density at the exit, and mass flow rate, and variability thereof, for the screw feeder identified in Objective 2 and the material properties measured in Objective 4. This model will be developed using the commercially available Abaqus software.
6. Experimentally measure the flow behavior of the powder identified in Objective 3 in the screw feeder identified in Objective 2. These measurements should take place at the IFPRI member’s facilities where the target screw feeder is available. Ideally, the graduate student working on this project would travel to aid in the testing, if additional funding support is available, e.g., through one summer internship provided by an IFPRI member. Alternately, IFPRI can provide the measurements via internal testing. The parameters to measure will include the mass flow rate, powder bulk density at the exit and, if available, screw torque or power. The screw should operate in volumetric mode during these tests in order to maintain a constant screw speed. In addition, if possible, the screw should be pulled out of the barrel during testing so that material build-up on the screw can be documented and compared to model predictions.
7. Using the continuum model developed in Objective 5, conduct parametric studies on the dependence of feeder performance on powder properties, e.g., internal friction angle, wall

friction angle, cohesion, hardening behavior, and system parameters, e.g., screw/barrel size and screw speed. The baseline properties will correspond to the screw feeder identified in Objective 2 and the material properties measured in Objective 4, and each parameter will be varied while holding the others constant.

Benefits to IFPRI members

The successful completion of this project offers several benefits to IFPRI members, in particular, and to the academic and industrial communities in general. These include:

1. Identification of promising feed screw designs, operating conditions, and material parameters relevant to controllable screw feeding.
2. More focused experimentation and a reduction in Design of Experiments testing for proper operation of screw feeders.
3. Improved process understanding.
4. Better control of screw feeder operation, its optimization and its scaling-up.

Schedule and Deliverables

Milestone (Deliverable)	Time from Project Start
Identification of screw feeder system and associated CAD drawings	Y1 – Q1
Identification of test powder	Y1 – Q1
Literature survey (written report)	Y1 – Q3
Powder mDPC properties (table of values)	Y2 – Q1
FEM-mDPC model development complete	Y2 – Q3
FEM-mDPC model predictions complete	Y2 – Q4
Experiment data measured	Y3 – Q2
Parametric studies complete	Y3 – Q3
Capstone final report (written report, Abaqus input and user files)	Y3 – Q4

Existing Activities at Purdue’s Center for Particulate Products and Processes (CP3)

The proposed research project could leverage on the following existing programs and research projects at Purdue’s CP3:

- a. Purdue’s “Pharmaceutical Engineering”, a Graduate Assistance in Areas of National Need (GAANN) grant from the U.S. Department of Education (supplement with 1/4 RA Ph.D. student)
- b. Purdue’s Particle, Powder, and Compact Characterization Laboratory (mDPC and other powder characterization equipment available)
- c. Purdue’s Rosen Center for Advanced Computing large scale computing clusters (both PIs have nodes on different clusters that will be used for the computations)
- d. Two U.S. Food and Drug Administration (FDA) grants titled “Advance regulatory science to support the implementation of continuous solid dose manufacturing systems, equipped with control systems that are capable of handling raw material variability and assuring product quality in real time” and “Industry 4.0 Implementation in Continuous Pharmaceutical Manufacturing” (opportunity to pursue the development of a mechanistic reduced order model, based on the predictive continuum model developed under IFPRI support, and use it for model-predictive control of Purdue’s Continuous Solids Processing Pilot Plant).

Budget

The total project budget is US\$38,000 per year for three years. This budget will be used to support a 1/4 RA Ph.D. student to perform the work, faculty time for guiding the student's work and managing the project, and laboratory expenses. Note that, as stated in the Proposed Objectives, the budget does not include the cost of making feed screw measurements at the IFPRI's member facility. If Purdue personnel are involved in this task, additional sources of funding will be needed in the form of at least one summer internship for the Ph.D. student involved in the project.

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