IFPRI Project Abstract

Single Droplet Drying at High Temperatures

Prof Andrew Bayly; Ph.D Students: Wael Ebrahim, Tien Nguyen
Institute of Particle Science and Engineering, School of Chemical & Process Engineering,
University of Leeds
Project Start Date: April 2016
Date: 1st June 2017

Project Objective:

This project seeks to develop experimental and modelling methods that enable dried particle structure, properties and drying rate to be predicted based on droplet drying history. The project will focus on effects driven by boiling and look to develop material independent models which capture behaviors of industrial interest. In particular it will look to address key limitations in current understanding: *1>* the impact of a non-isothermal drying history on particle structure and consequently drying rate; *2>* improved measurements of material properties under the non-equilibrium conditions experienced during drying; *3>* extension of models to include the mechanics of structure formation.

Approach:

Initially, material classes and materials will be identified. Novel experimental rigs and methods will be developed to allow unsteady drying behaviour to be investigated and material properties to be measured under relevant conditions. Established models will be extended to include better material models and mechanical deformation. We will bring this together into a regime map(s) which links material properties, particle size, initial moisture content and drying history to morphology.

Recent Results:

Resources and group establishment: Modelling PhD student started; complementary EPSRC project kicked off; ADDOPT project (focusing on crystallization) in progress.
Experimental development for regime mapping: Mono-dispersed atomizers for drop tube evaluated and Leeds nozzle selected; Dryer/drop tube performance further benchmarked, CFD model of dryer developed; Single droplet filament rig built, droplets successfully imaged, method development in progress to enable experimental mapping.
Material properties: Microwave drying rig for rapid material property evaluation evaluated and discounted.
Modelling: Droplet drying modelling methodology evaluation underway.
Regime Map: Approaches developed for theory/model based regime map initiated.

Next Steps:

Priorities are: evolution and method development of **drying rigs** for experimental mapping; Development and evaluation of novel techniques for **material property** characterization. **Resolved model** for bubble growth and structure development, starting with viscous material model, initially 1-D then 3-D with external flowfield.

IFPRI Project Abstract

Nonlocal Rheology of Intermediate Granular Flows: Particle Shape and Size Distributions

Zhu Tang, Ted Brzinski, Michael Shearer, Karen Daniels
Dept. of Physics, NC State University, USA
Project Start Date: 10 August 2015
Abstract Date: 19 May 2017

Project Objective:

Our research aims are to connect grain-scale parameters to macroscale behaviors within a sheared granular material, through the use of a nonlocal rheology. We aim to answer 3 questions: (Q1) What do the flow field and fluidity field look like for real experiments? (Q2) How do the empirically-measured material properties and cooperativity length vary as we change particle shape and size and distributions in a controlled way? Do these properties help distinguish the competing models? (Q3) Can the fluctuations in local forces (via force chains breaking/forming) account for the non-local contribution to the fluidity?

Approach:

We perform experiments in a quasi-2D annular shear cell [1], in which tracking the locations and velocities of individual particles is possible. This allows for direct tests of two competing nonlocal theories [2,3] which so far have seen little experimental validation. The present work focuses on testing whether these two models can successfully explain the observed velocity profile $v(r)$ and rheological behavior $\mu(I)$. In particular, we seek to uncover what features distinguish the two models. At present, we have focused on a single set of particles, but have started to laser-cut more complex shapes for use in ongoing work. Ultimately, the use of photoelastic particles will permit measurements of the full pressure field and its fluctuations.
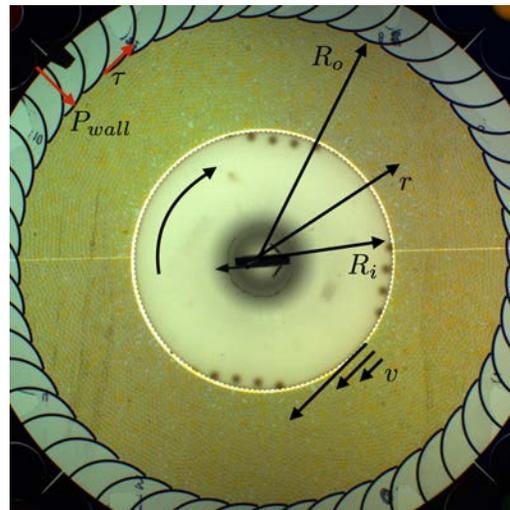

Figure 1: Top view of apparatus, with leaf springs around outer confining wall. The inner disk rotates, shearing the granular material (~ 10^4 particles).

Recent Results:

We have calibrated the outer leaf springs (see Fig 1) so that they can measure both the normal and tangential stress at the outer wall. This technique has been accepted for presentation at Powders and Grains 2017, and a paper will appear in the proceedings [1].

We have used these measurements, in combination with creating an empirical model for the basal friction, to make quantitative comparisons to the two nonlocal models [2,3]. We find that at two different packing fractions and for 4 rotation rates spanning 3 orders of magnitude, both models can capture the observed relationship between the stress ratio (shear stress/pressure) and the inertial number, answering Q1 above. A single set of parameters (for each model) successfully provides agreement for all six runs. However, we find that the nonlocal length scale ξ diverges at the yield stress ratio μ_s, which is a feature of only one of the two models [2].
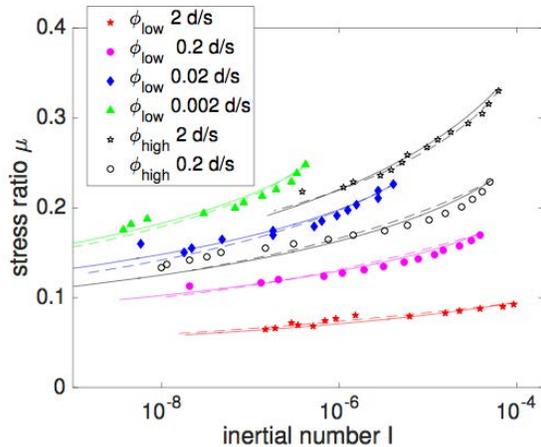

Figure 2: Rheological measurements from six different experiments (symbols), compared to modelling via the cooperative model [2] and the gradient model [3].
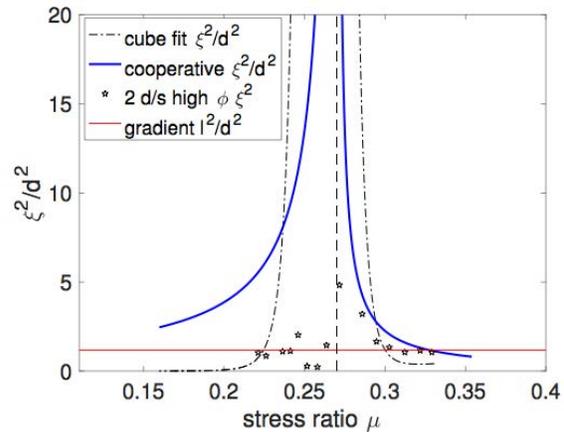
Figure 3: Measured length scale (symbols, dash-dotted line) compared to predictions from the cooperative model [2] and the gradient model [3]. Divergence is at yield stress.

Next Steps:

We will collect data on how different particle shapes (or other properties) effect the model parameters (Q2) and the choice of model [2,3]. We will determine what generalization about the material properties is possible, and which shape/size properties are the most important to characterize in a simplified description. We will also begin to implement the tracking of the internal stress field, through the use of photoelastic particles, to more directly test the origins of nonlocality (Q3).

References:

[1] Z.Tang, TA Brzinski, and KE Daniels. "Granular rheology: measuring boundary forces with laser-cut leaf springs." *Powders & Grains 2017* http://arxiv.org/abs/1704.08295

[2] K Kamrin and G Koval. "Nonlocal Constitutive Relation for Steady Granular Flow." *Physical Review Letters*. 108, 178301 (2012)

[3] M Bouzid, M Trulsson, P Claudin, E Clément, B Andreotti, "Nonlocal rheology of granular flows across yield conditions." *Physical Review Letters*. 111, 238301 (2013)

![IFPRI logo] **IFPRI Project Abstract**

Creating Tuneable Agglomerates via 3D Printing

Prof. Karen Hapgood[1,2] & Mr Ruihuan Ge[1] (PhD student) in collaboration with Dr Zongyan Zhou[1] and Prof. Mojtaba Ghadiri[3],
[1]Monash University, Australia; [2]Deakin University, Australia; [3]Leeds University, UK
Project Start Date: 01 Jan 2015
Abstract Date: 26 May 2017

Project Objective:

To produce systematically varied or "tuned" agglomerates with controlled properties structure, and validate simulation models of granule breakage.

Approach:

Agglomerates with defined and tuneable properties were produced using 3D printing technology. Quasi-static and impact breakage tests were conducted to vary strain rate under controlled conditions. Macroscopic agglomerate breakage experiments were compared with DEM simulation results to validate the newly developed Timoshenko Beam Bond Model (TBBM) contact model.
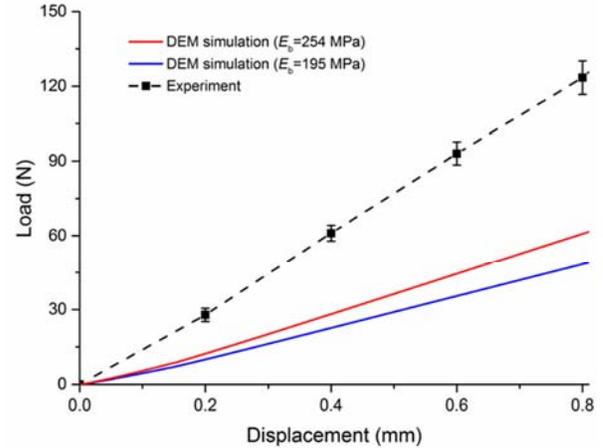

Recent Results:

Qualitative comparisons of the failure mode between experiment and DEM simultiosn (using TBBM bond model) were successful, after experimentally measuring the strength of the inter-particle bonds and using the data to extract the Youngs modulus.

Simulation (E_b=195 Mpa)

Experiment
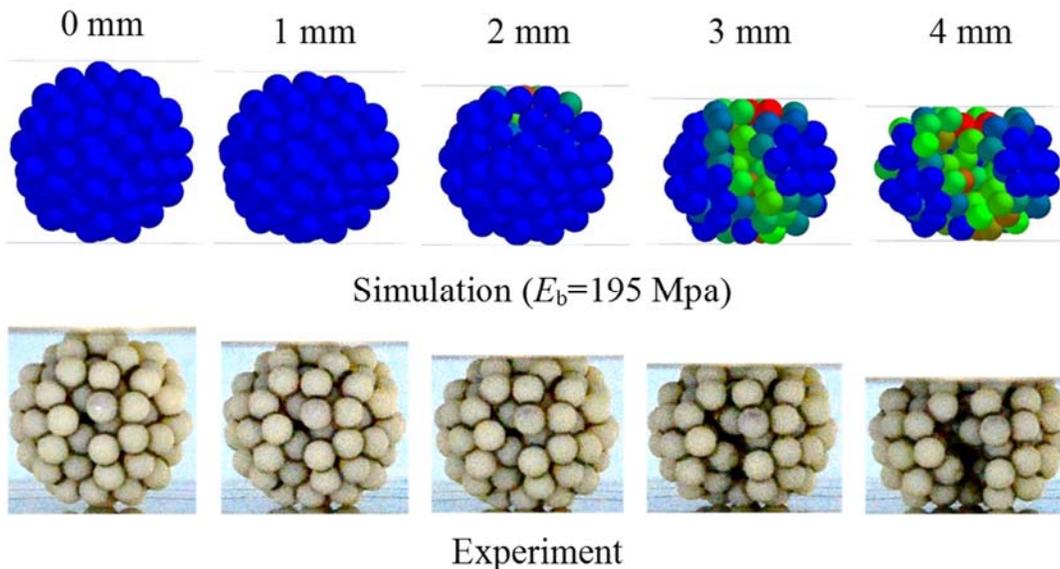
The quantitative load-displacement results shown that DEM simulation was an excellent match for the cubic tetrahedral agglomerate structure (left). However, DEM underestimated compressive loads for spherical random agglomerates (right) that can be attributed to TBBM bond geometry definition differences and non-linear polymer behavior.
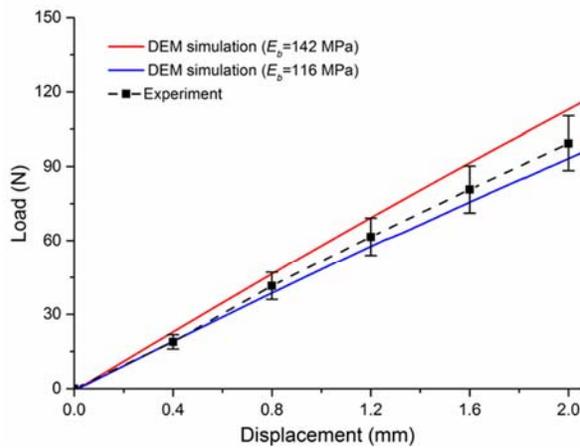
(a) Cubic tetrahedral structure   (b) Spherical random structure

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Next Steps:

Complete and write up the DEM and experimental comparisons.

Obtain XRT scan of a real granule (non-spherical particles) and print and conduct breakage tests.

Final IFPRI report

Flowability Assessment of Weakly Consolidated Powders

Colin Hare[1], Ali Hassanpour[2]
[1] Department of Chemical and Process Engineering, The University of Surrey, UK
[2] School of Chemical and Process Engineering, The University of Leeds, UK
Project Start Date: 05 March, 2015
Abstract Date: 19 May, 2017

Project Objective:

Measurement of unconfined yield strength of powders can be made with a variety of commercially available shear testing devices. Traditional flowability measurement devices have a number of short comings, e.g. reproducibility of unconfined yield strength is greatly reduced at low stresses, sometimes measurement is inconsistent with observed behaviour, or materials found to be cohesionless may still have practical differences. Generally the onset of flow is measured, which may not be a complete flow description. IFPRI seek to develop a theoretical understanding of flow of weakly consolidated and weakly cohesive powders.

Approach:

We adopt the ball indentation method for determining powder flowability by measuring the resistance of a powder bed when penetrated by a sphere which is quasi-statically introduced. It is necessary to determine the constraint factor of a powder in order to infer the yield stress from the indentation measurement. Indentation measurements are compared to shear cell measurements at the same major principal stress, for a range of moderate stresses, in order to determine constraint factor. The influence of single particle properties on constraint factor is explored in order to be able to predict its value so that indentation alone can be used to infer the yield stress.

Recent Results:

Previous results showed that for a number of powders the constraint factor varied notably with major principal stress. Analysis of the yield locus and failure mohr circle generated by the shear cell, for each tested stress for all materials, indicated that in many cases the range of applied normal stresses led to the yield locus being extrapolated significantly in order to determine the failure mohr circle, and hence the unconfined yield stress. Shear cell measurements have been repeated for these powders with more suitable applied stresses, therefore removing the need to extrapolate the yield locus. For several measurements this led to a change in unconfined yield stress, when compared to the previous (inaccurate) value. As a result, the constraint factor is now found to be

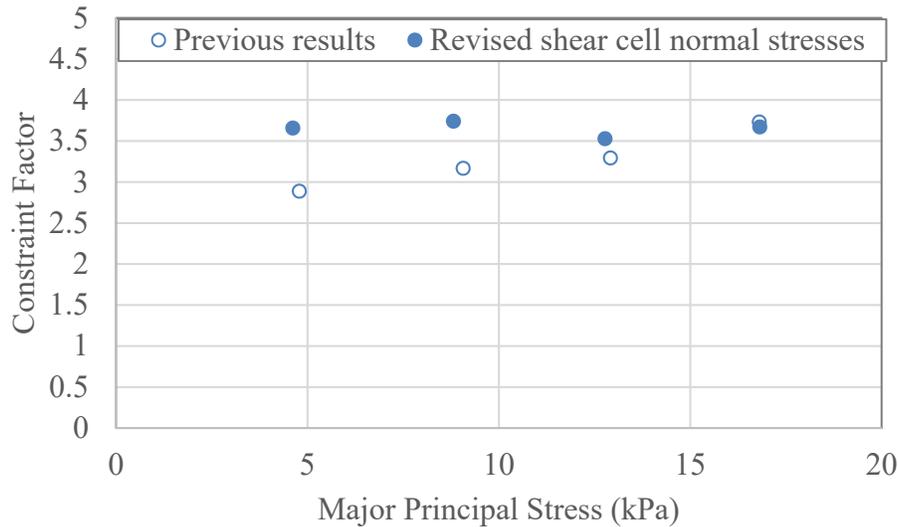independent of major principal stress for most materials; this is demonstrated for maltitol in Figure 1.

Figure 1. Revised Constraint factor values for maltitol

Measurements with five consecutive single sieve cuts of silanised glass beads suggest that constraint factor shows a slight reduction as particle size is increased. Results using size distributions with fixed median size but varying span ($[d_{90} - d_{10}]/d_{50}$) indicate that the width of size distribution has no significant effect on constraint factor.

For the 45-53 μm silanised glass beads the shear cell generates reproducible and seemingly reliable yield loci at remarkably low pre-shear normal stresses of $0.1 – 1$ kPa. In this stress range the unconfined yield stress changes more dramatically with major principal stress than at higher stresses, as indicated by the ball indentation measurement. It is noted however that unconfined yield stress inferred from the ball indentation measurement is greater than that determined from the shear cell.

Next Steps:

The influence of surface energy on constraint factor will be assessed using glass beads silanised with different functional groups, and the shape effect will be assessed with three different copper samples. A statistically reliable prediction of constraint factor based on particle properties is required to apply the ball indentation method, and hence a large number of varying powder samples must be considered. Constraint factor could be determined using unconfined yield stress measurements from shear cell or uniaxial compression tests; the optimal method needs to be determined. Furthermore, the variation of packing fraction in the failure zone in these two techniques, and in ball indentation, should be explored.

IFPRI Project Abstract

Powder Structure Control

J. Harnacke, R. Kohlus
Universität Hohenheim, Stuttgart, GERMANY
Project Start Date: [1.January 2015]
Abstract Date: [26 May, 2017]

Project Objective:

Finding the best numerical descriptors of powder structure and understanding how they relate to relevant powder properties, e.g. dissolution, dispersing, strength and compactability. This requires developing an understanding of the mathematical meaning of structure descriptors and their relation to physical meaning, i.e. connectivity, interface prediction, correlation length and voidage. Additionally, the best descriptors for a given purpose, e.g. either prediction/modelling of product characteristics or control of structure generation shall be given.

Approach:

The basic approach of the project assumes, that granule structure, i.e. two phases plus porosity, can be quantified based on spatial statistics, e. g. covariance functions and linear path distances. For measuring structure, x-ray micro tomography is used to generate 3D images that are analyzed using point and line statistics. Variation in granules structure includes type of structure (random layered, clustered) and various amounts of porosity.

Recent Results:

The property function of powder structure (average particle-particle distance) to dissolution behavior was extended to small minimal particle distances. Sintered , highly porous as well as fluid bed agglomerated systems has been included in the assessment of structure property correlations. Single particle dissolution was modelled by a 3D diffusion approach based on XRT structure measurements. Finally an impact attrition test (Malvern, Scirocco) has been applied successfully as an additional strength measure for the structured powders.

Next Steps:

Completing the study with attrition test by impact and compare to single particle crushing results. A high number of systematic runs of the structure depend dissolution simulation will be performed to get statistically relevant results. Parallel a summary report about powder structure will be compiled and prepared as final project report.

IFPRI Project Abstract

Quantitative Prediction of Segregation at Process Scale

Joseph J. McCarthy
University of Pittsburgh
Project Start Date: 1 September 2015
Abstract Date: 13 May 2017

Project Objective:

This project is aimed at identifying critical material and process parameters that control the extent of powder segregation, such that we might develop quantitative models that predict segregation. These predictive models should be valid at full process scale and are to be validated against appropriate experiments.

Approach:

Segregation rate models hold promise for scale-up via continuum-level analysis using device-specific transport equations; however, experimental validation of dynamic models is extremely difficult and typical segregation models are not inherently built with scale-up in mind. Our approach overcomes the experimental limitation by exploiting competing time-scales in artificially forced granular flows to establish a unique "equilibrium" between mixing and segregation. With regard to the scale-up limitation, we have built – and plan to continue building – segregation models that are written expressly in dimensionless form with an aim at both connecting segregation modeling to flow rheology as well as enable more transparent scale-up. We are using our experimental segregation validation framework both to benchmark existing segregation rate models as well as to test our new and developing models.

Recent Results:

Our most recent successes include establishing the first analytical connection between density-based segregation to granular rheology. This model is based largely on first principles and fits data from a variety of boundary conditions, density ratios, shear rates, gravitational conditions, and material properties. Moreover, we have begun building complementary segregation models for size, shape, and cohesive segregation and have validated our shape model.

Next Steps:

In our second phase of IFPRI funding we anticipate completing our modeling efforts for size, shape, and cohesive segregation. In addition, we expect to continue additional experimental validation of these models. Finally, we plan to incorporate our newly developed models into transport equations to enable large-scale validation against process-scale data.

IFPRI Project Abstract

A Holistic Approach for the Model-based Control of Crystal Size, Shape and Purity in Integrated Batch and Continuous Crystallization - Wet Milling Systems

Zoltan K. Nagy
Purdue University, Davidson School of Chemical Engineering, West Lafayette, US
Project Start Date: ??????
Abstract Date: 01 05, 2017

Project Objective:

[2-3 sentence summary of original project brief]
The main objective of this project is the design of novel, integrated crystallization systems, which are supposed to produce wider variety of crystalline materials, in the context of crystal size and shape distribution as well as purity. The attainable region of crystal size distribution (CSD) is widened by the application of recirculation stream as well as by integrating wet mill for batch, and multiple MSMPR units and downstream wet mill with recirculation stream(s) for the continuous operation. Growth rate modifiers are also considered for crystal size and shape, as well as for purity control.

Approach:

[2-3 sentence summary of project proposal (experimental/theoretical approaches)]
Model based approaches are intensively applied, namely the population balance (PB) framework. 1D and 2D PBM-s will be developed for the batch and continuous integrated systems, involving the high resolution finite volume method (HR-FVM) for the solution of generated model-equations. In solver implementation advanced compute infrastructures, such as parallel calculations on low-cost and high performance GPU accelerators, are involved for the sake of creating generic numeric solution platforms for the aforementioned systems. Novel, iterative model-based experimental design (IMED) will be used for optimal estimation of the parameters of generated models.

Recent Results:

[Short summary of past year's progress and its significance, including one or two illustrative graphics (if useful)]
Generic solvers for 1D and 2D batch and MSMPR systems have been created, with and without GPU acceleration. The numerical performance of these implementations, in the context of simulation time and accuracy, has been deeply studied. For extreme cases, the GPU acceleration in 2D PBM solution delivered 2 order of magnitude speedup over the serial C implementation, which, under the same conditions, was by 2 orders of magnitude

faster than the corresponding MatLab simulation. Using these efficient codes, the first version of a generic crystallization platform has been created, with a MatLab based function and a generic GUI, called as CrySiV, for the acronym of Crystallization Simulation and Visualization tool.

Soft-sensors for the PVM and FBRM were also created for prism-like and cube-like crystals.

An integrated batch crystallizer-wet mill model, involving 1D PBM was created, numerically evaluated and used for simulation and optimization of the product CSD.
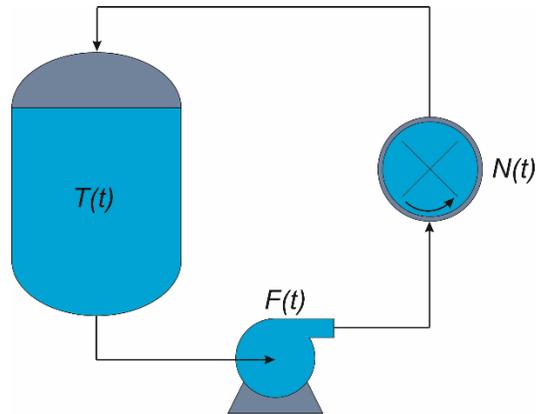

Figure 1. Integrated batch crystallizer-wet mill system with the most important design parameters (temperature, circulation flowrate and wet-mill revolution speed)

The preliminary optimization results clearly showed that in optimal operation the external wet mill is used as an in-situ seed generator while the pump ensures the optimal dynamic seed addition. With these two features the product CSD can be arbitrary tuned, of course, only within the attainable CSD domain.
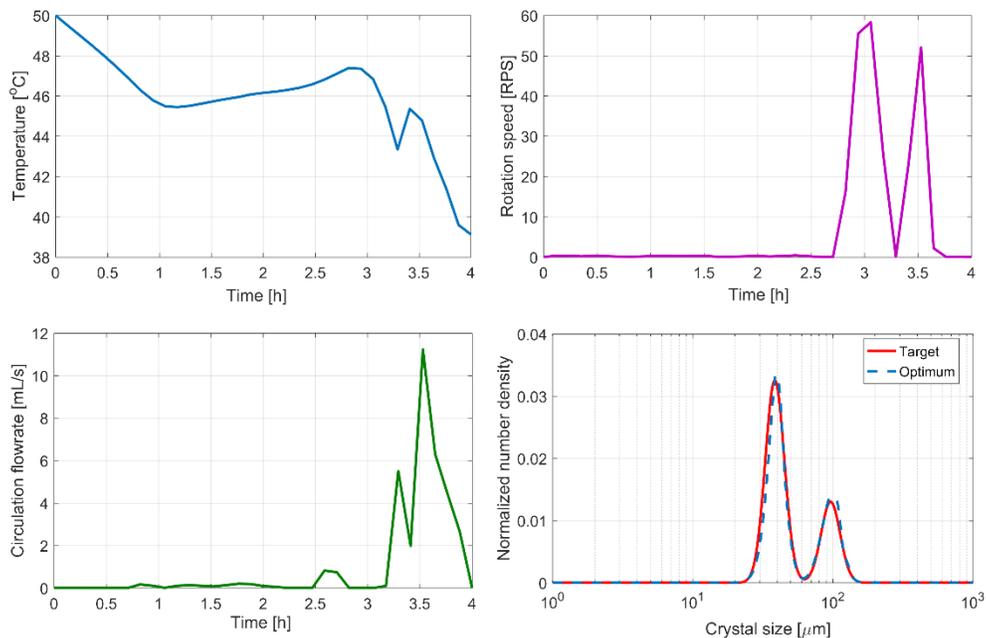
Figure 2. Preliminary optimization results for the production of bimodal CSD in batch operation

Next Steps:

[2-3 sentence summary of where the project is headed in the next year. If the project is in its last year, a short summary of open questions.]

In the next year the PVM and FBRM soft sensors will be extended to cylinder and sphere shape crystals as well as the artificial neural network simulation of the two instruments will also be worked out.

In the line of process modeling, the integrated system will be extended to 2D continuous case, using which numerical analyses and optimizations will be carried out.

Progress will also be made on the estimation of 1D integrated system as well as implementation of predictive control for 1D and 2D batch crystallization processes.

The extension of the CrySiV GUI, as well as its generic PBM solver function counterpart will be continued.

IFPRI Project Abstract

Milling and Material Grindability

Jin Y. Ooi, Lige Wang, Xizhong Chen, Jin Sun, Jian-Fei Chen*
University of Edinburgh, U.K.; * Queen's University Belfast, U.K.
Project Start Date: 07 January 2013
Abstract Date: 12 May 2017

Project Objective:

This project aims to develop a robust methodology to characterize the grindability of particulate products in milling operations. This involves developing grindability measures to characterize the comminution of particulates. The measures, when coupled with milling function through computational modelling, will be used to predict milling processes.

Approach:

1. Explore the population balance model (PBM) in comminution process and conduct PBM simulation to predict the product size distribution under varying operational conditions.
2. Conduct multiscale analysis of DEM simulation at particle scale and further coupled with PBM at process scale to inform the milling behavior in an impact pin mill;
3. Develop the material function: characterize particle breakage subjected to the dominant loading events identified within a milling operation.

Recent Results:

1. A multiscale DEM-PBM coupling framework was proposed to predict the milling behavior of particles in an impact pin mill.
2. The selection and breakage functions in the population balance model were explored by upscaling the information from lab scale to process scale.
3. The predicted product size distribution via PBM shows good agreement with milling tests under four rotary rates.

Next Steps:

The project will progress next year with emphasis on the parameters estimation in the selection and breakage functions in the population balance model with further impact tests at higher impact velocity or a properly calibrated bonded contact model. The coupling of PBM with DEM will be applied to predict the product size distribution beyond the current experimental space.

On the long-term stability of colloidal gels (2)

Wilson Poon
The University of Edinburgh
Project Start Date: 1 October 2016
Abstract Date: 15 May 2017

Project Objective:

A new paradigm for colloidal gel collapse emerged from our first project involving dense 'debris' accumulating at and then falling from the top and solvent bubbles rising from the bulk coupled with hydrodynamic back flows. In this three-year extension project, we propose to elucidate the origins of the falling debris and rising solvent bubbles, explore whether other mechanisms exist in other regions of parameter space, and study in detail in the role of hydrodynamics in all processes relevant to triggering gel collapse.

Approach:

Experimentally, we propose to continue to base most of our work on the model system developed during the first three-year project, but changing a number of parameters not hitherto explored (e.g. the range of the inter-particle attraction) and adding complexity (e.g. including two sizes of particles). Computer simulations will be performed using the Lattice Boltzmann method to take into account the solvent flow. One advantage of our approach is that all parameters for the experiments are known, therefore facilitating direct comparison with simulations.

Recent Results:

Experimentally, we have found that eliminating the top meniscus with air in our gels significantly affect their 'shelf life', probably because without a curved air-gel meniscus, few, if any, heavy 'debris' accumulate at the top. Instead, rising solvent 'bubbles' destroy the gel structure. Computer simulations with hydrodynamics have found that gels with larger particle sizes age more rapidly. We have also obtain the first results showing how the rise of a solvent droplet destroys gel structure via back flow.

Next Steps:

We plan to complexify our experimental system by including particles of two different sizes. Such a system may simulate, e.g., a product where a small-particle colloidal gel matrix holds up larger particles. Large-scale 'production runs' from our simulations will explore systematically how and why particle size affects gel aging.

IFPRI Project Abstract

Self-Assembled Monolayers as Nucleating Surfaces to Study Early Formation Pathways of Crystal Polymorphs

Ulrich Wiesner

[Materials Science and Engineering, Cornell University]

Project Start Date: [15 September, 2015]

Abstract Date: [15 May, 2017]

Project Objective:

In order to establish scientific correlations between nucleation and observed polymorph, in particular to polymorphs not accessible via solution methods, we have chosen heterogeneous surface nucleation via SAMs as the primary means to study polymorph selection.

Approach:

We have used self-assembled monolayers (SAMs) as well-defined surfaces that can be used to study the relationship between the nucleation event and the final polymorph selection. Furthermore, by tuning the substrate-crystal interface energy, potentially crystalline order of SAMs can promote the nucleation of polymorphs not accessible via solution methods. This year we have expanded the variety of SAMS substrates and chemistries to include silane-silica systems, which offer a greater variety of surface chemistries, transparent substrates for in-situ optical studies, and overall less expensive materials.

Recent Results:

We have found that both solvent and substrate work together to control crystal polymorph. On hydrophobic SAMS, pure solvent systems such as ethanol, water, and 1,4-dioxane yield the thermodynamically stable, monoclinic polymorph of acetaminophen (ACM). However, mixtures of water and 1,4-dioxane produce the less favored orthorhombic form. While some solvent produce the same polymorph on both hydrophilic and hydrophobic SAMS,

Furthermore, the surface chemistry of the SAM can strongly influence the orientation of the nucealtion and crystal growth. For example, for a given solvent, hydrophobic surfaces promote the orthorhombic form of ACM with the (002) cleavage plane perpendicular to the substrate, and the -OH surface induces the same orthorhombic polymorph, but with the (002) plane parallel to the substrate. We hypothesize that this selection is due to the

energetic favorability of certain crystal facets interacting with the chemically specific SAMs surface. (See Figure 1).
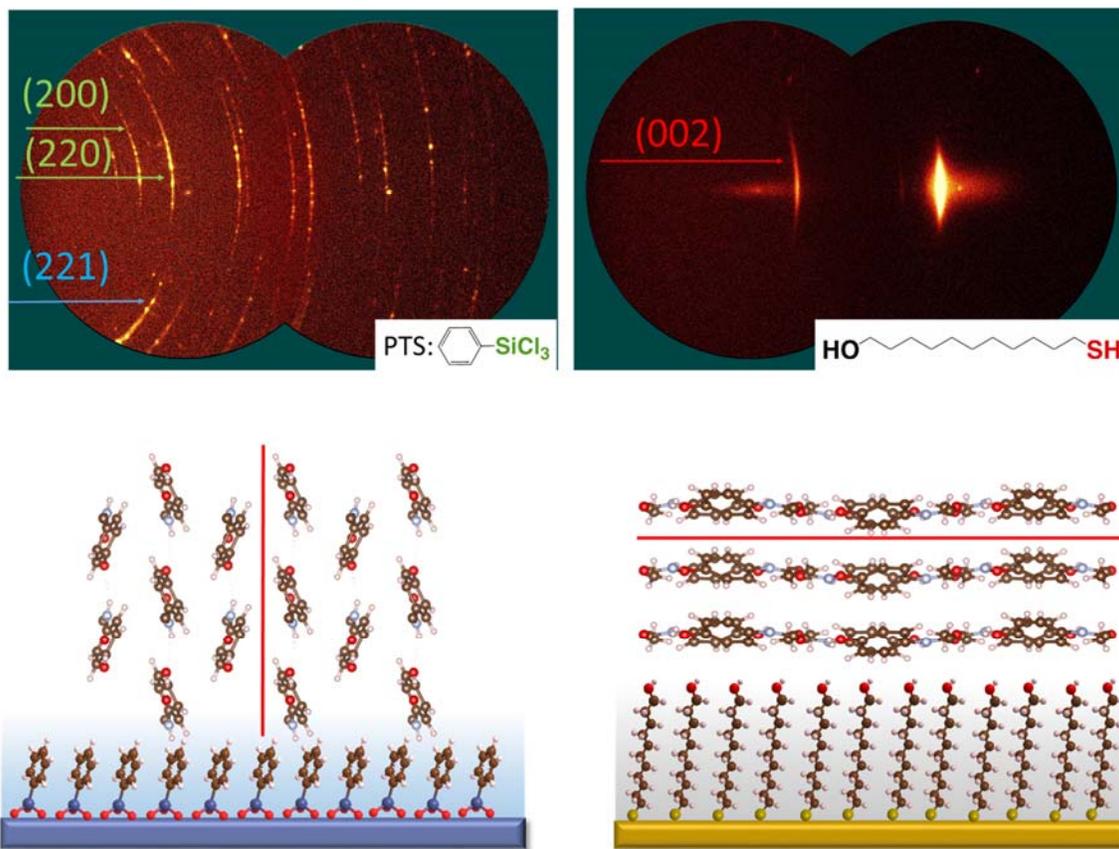

Figure 1. Clockwise from top right: x-ray diffraction pattern of orthorhombic ACM crystallized on hydrophobic surface (PTS). X-ray diffraction pattern of orthorhombic ACM crystallized on hydrophilic surface (-OH). Molecular interpretation of how ACM crystal is oriented on -OH SAM. Molecular interpretation of how ACM is oriented perpendicular on hydrophobic PTS SAM. The two surfaces yield the same polymorph yet vastly different crystallization orientations.

Next Steps:

Using the silane-based SAMS we have developed in the last year, we have recently begun blade coating solutions of ACM onto silica substrates. This approach will allow us to utilize Cornell's High Energy Synchrotron Source (CHESS) to study the early crystallization processes by x-ray diffraction *in-situ*. Moreover, blade-coating introduces the potential for further influencing the polymorph selection through shear force.

IFPRI Project Abstract

Die Filling of Aerated Powders

Prof. Chuan-Yu (Charley) Wu
Department of Chemical and Process Engineering, University of Surrey, Guildford, GU2 7XH, UK

Project Start Date: 01 November 2016
Abstract Date: 19 May 2016

Project Objective:

1) *to explore fine powder mixtures during die filling processes encountered in real manufacturing process;*
2) *to identify the critical material attributes and critical process during die filling of aerated powders; and*
3) *to develop a design space for fine powder mixtures to achieve controlled/specified properties during die filling (such as mass variation, content uniformity, mass flow rate).*

Approach:

It was proposed to experimentally explore the following 3 aspects: 1) rotary die filling, for which a model rotary die filling system is developed and powder flow behavior during rotary die filling will be explored systematically. 2) assisted die filling, for which suction filling and die filling with paddled hopper/shoe will be developed, and systematic experimental study will be performed; 3) Segregation during die filling. Both size-induced and density induced segregation will be explored.

Recent Results:

A rotary die filling system (Fig.1) was constructed and used for exploring die filling behavior of a wide range of materials. The die filling behaviour was also compared to that of linear die filling. It was found that the filling efficiency is significant improved with rotary die filling (Fig.2).

In addition to size induced die filling reported in the last AGM, density-induced segregation in the shoe and in the die was explore. It is shown that significant segregation can take place during die filling (Figure 3).

In previous project, it was noted that there was a dramatic air pressure change in the die during die filling. Further mechanistic analysis was performed that the air pressure change in the die can be well predicted using a transient die filling model (Figure 4)

The dependency of die filling performance on powder flowabiloty was also explored. It was found that there is a strong correlation between die filling performance and the flow index measure using Flodex (Figure 5).
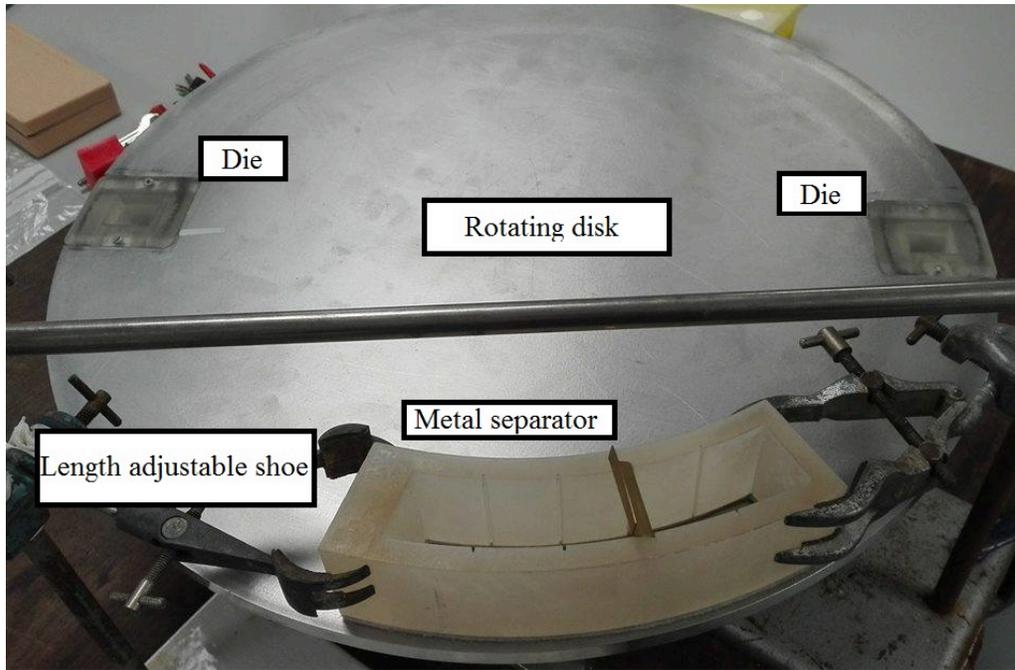

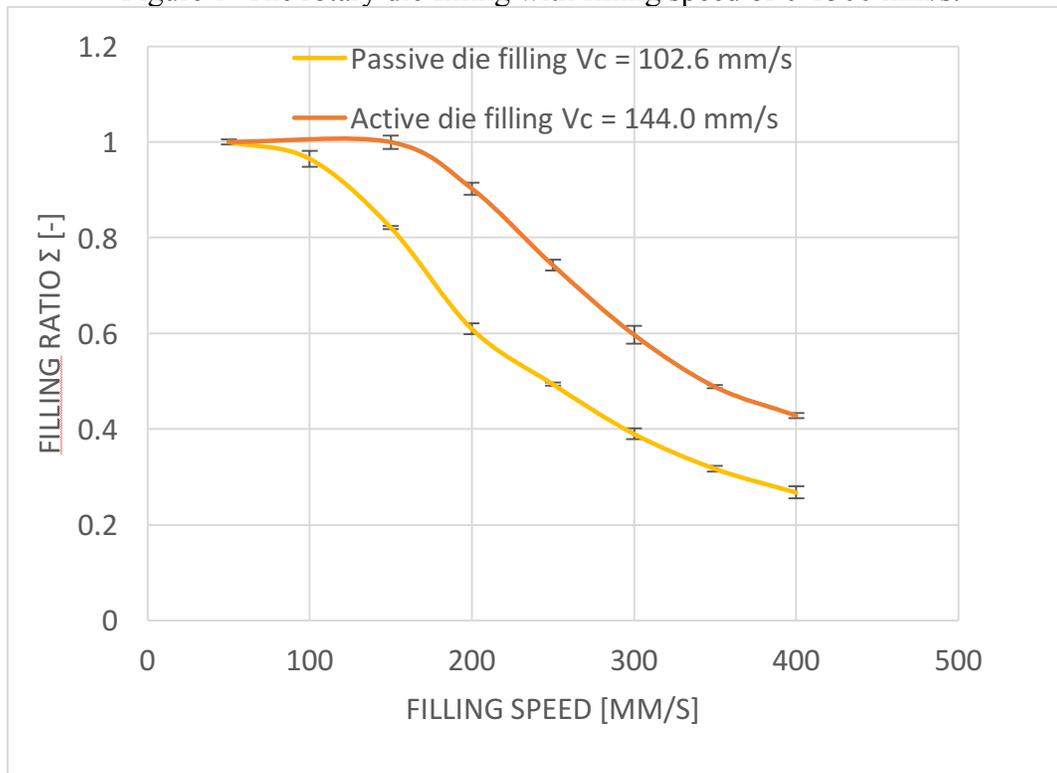Figure 1 The rotary die filling with filling speed of 0-1500 mm/s.

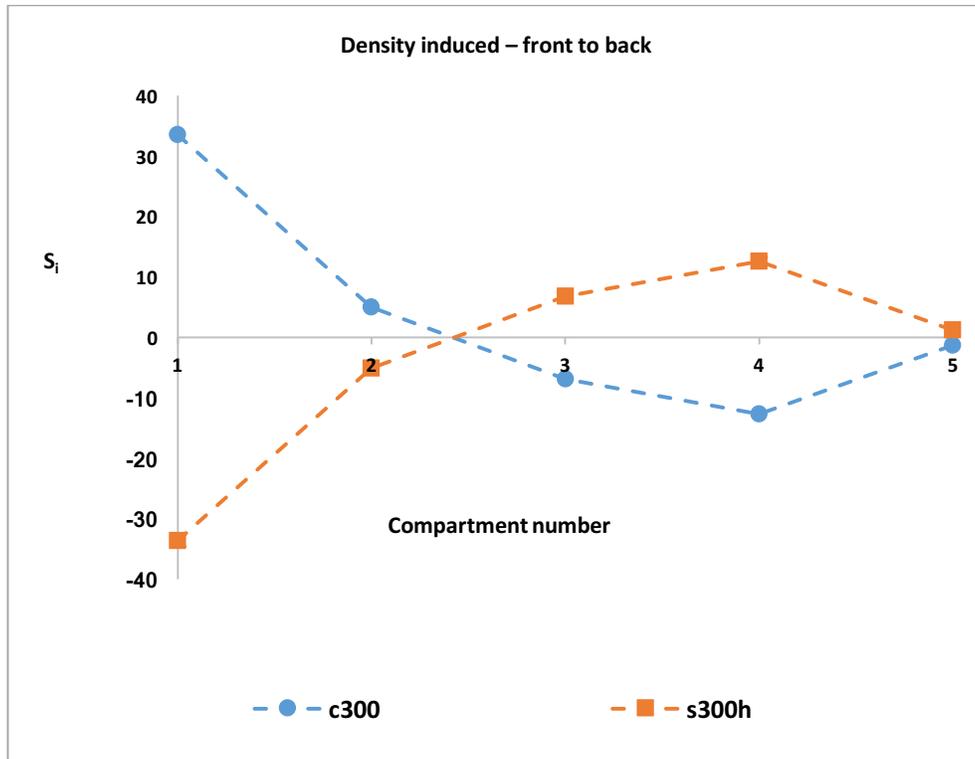Figure 2 Rotary die filling (Active) versus linear die filling (Passive)
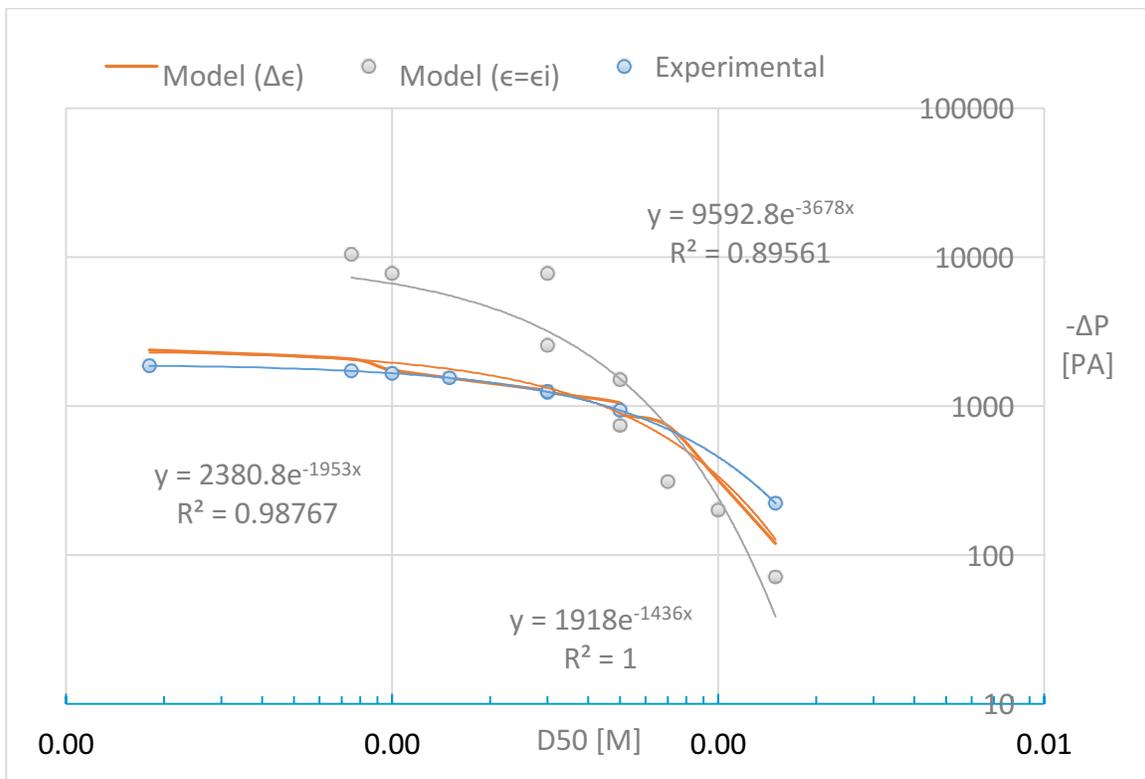
Figure 3 Density induced segregation.

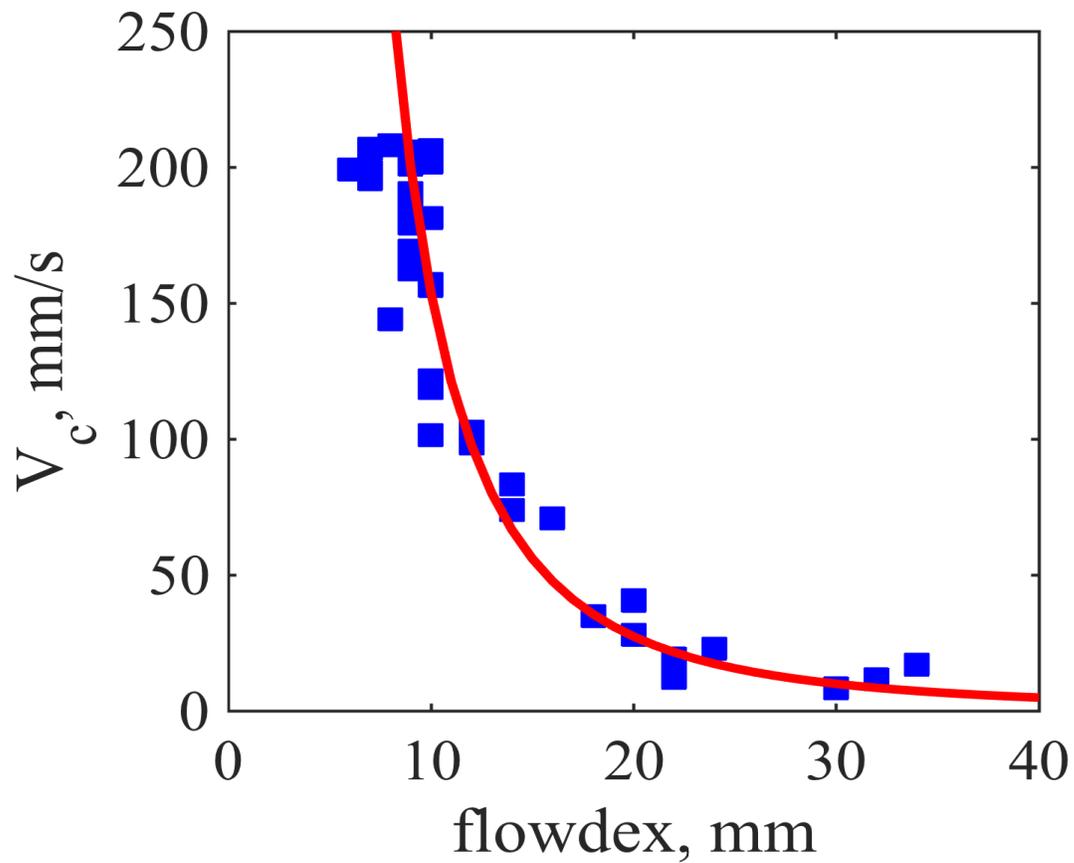Figure 4 air pressure change during die filling.

Figure 5 Critical filling speed versus flow index.

Next Steps:

The following future work is planned
1) Suction filling: system development and detailed experimental investigation;
2) Paddled hopper/shoe: system development and preliminary investigation;
3) Correlation with other flow measurements;
4) Further Rotary die filling study – Moist/cohesive powders.

IFPRI Project Abstract

Multiscale Modeling of Compaction with Emphasis on Powder Mixtures

Antonios Zavaliangos
Department of Materials Sci. & Eng ., Drexel University, Philadelphia, PA19104, USA
Project Start Date: [2012]
Abstract Date: [25 May, 2017]

Project Objective:

This project focuses understanding the compaction and strength of powder mixtures. Multicomponent formulations are pervasive across diverse industries and understanding aspects of their behavior through modeling with minimum experimentation is highly beneficial, because the experimental matrix that addresses all potential combinations of variables is rather daunting.

Approach:

Modeling of multi-component systems using discrete element method (DEM) is a natural way to approach this complex problem, because the experimental matrix that address all potential combinations of variables is rather daunting. Modeling validated with experiments is the methodology that will provide us with insight into the cause of the various effects and can delineate the relative importance of multiple, coexisting factors. However, existing models are based on force-displacement laws that describe only small deformations, and no work exists for dissimilar materials.

Recent Results:

Major efforts during this year included (a) exploring appropriate definitions for damage so that we can quantify propensity for failure, (b) visualization of damage, (c) testing the ability of the single material model to reflect material properties by comparing model parameters for non-lubricated and lubricated materials, (d) understanding the effect of residual stresses on the strength of mixtures.

Next Steps:

Identification of the model weaknesses. Validation of the model using appropriate model mixtures. Evaluation of residual stresses in powder mixtures using x-ray diffraction.