PROJECT BRIEFS FROM 2015

IFPRI International Fine Particle Research Institute

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Control/Manipulate Powder Surface Properties and Additives for Wetting and Incorporation
1.1	Project / Review	Project
1.2	Technical Area	Wet Systems
2.0	Submitted by	NJ Wagner
2.1	Member company/ies	Syngenta, Johnson Matthey, DuPont, P&G
2.2	Idea creation date	June 22, 2015
2.3	Last modification date	
3.0	Short goal description	Control and manipulate the molecular and nanoscale properties of powders and the optimal design of surface modifiers for ease of incorporation and rheology evolution
3.1	Objectives	1. Control/manipulate/engineer nano to meso scale powder surface topology to promote wetting and powder incorporation/dispersion into liquids 2. Control/manipulate/engineer powder surface chemistry to promote wetting and powder incorporation/dispersion into liquids 3. Optimize/minimize the use of surface modifiers, such as surfactants, potential determining ions, polymers, to promote wetting and powder incorporation/dispersion into liquids 4. Objectives 1-3 above focused on achieving a desired rheological state 5. Develop rheological methods to aid in objectives 1-4.
3.2	Scope	Incorporation and dispersion of powders into solutions often requires energy to cross the air/liquid interface and immerse into the liquid. Powder surface properties can benefit by nano and mesoscale control of topology and chemistry to promote wetting, incorporation, and dispersion. Additives such as surfactants, ions, and polymers as well as combinations thereof, are often used to promote incorporation and dispersion. Optimal design and choice of surface modifiers will be considered with regards to powder properties. A broad range of materials are to be considered, including inorganic and organic particles, including bioderived materials. Finally, the effects of these methods of incorporation and dispersion on rheology, including time-dependence, are to be considered.

		Out of Scope: Use of high energy input to the system.
4.0	Contractor	Paul Chaiken (NYU), Lucio Isa (ETH-Zurich), Kate Stebe (U Penn)
4.1	Comments / experiences	JM: powder incorporation differences between powders

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Interaction of Material Response and Milling Process in Defining Grindability
1.1	Project / Review	Project
1.2	Technical Area	Size Reduction
2.0	Submitted by	Mojtaba Ghadiri on behalf of Size Reduction Group: Chris Rueb, Jeff Hoffmann, Gary Liu, Joe Atria, Marcelo Tavares, Jim Davis, Paul Mort, Jin Ooi, Charles Compson, Ed Durham, Maxx Capece, Hugh Stitt
2.1	Member company/ies	Johnson Matthey, Du Pont, Almatis, Aveka, Paul O Abbe, Powder, Evonik, AbbVie
2.2	Idea creation date	23 June 2015
2.3	Last modification date	
3.0	Short goal description	• Establish grindability for a wide range of material properties by considering the prevailing stress regime ranging from collisional to rapid shearing systems, as in pin mills, hammer mills and roller crushers. • Build a grindability map that shows the connection among material properties, targeted product particle size distribution and milling stress conditions.
3.1	Objectives	1. Provide mechanical properties for Edinburgh's program. Need to ask what key information is missing. Shear strength, particle density, hardness, etc. along with bulk material properties such as bulk density, a flow function, bulk cohesion etc. Overall there is a great need for characterization of the materials so that the effects can be better understood. 2. Understand material response, particularly for semi-brittle materials in terms of strain rate sensitivity, moisture content. 3. Connect materials characteristics and milling stress conditions both via impact and shear stresses …this is where the DEM can be very useful for comparison.
3.2	Scope	Carry out a project which is complementary to the current project at Edinburgh, benefitting from DEM work ongoing there and providing material-related information for it, and at the same time developing material-oriented grindability methods on final targeted product particle size distribution.
4.0	Contractor	Luis Marcelo Tavares, Haim Kalman, Ben Gurion,

		Stephan Heinrich, Hamburg
4.1	Comments / experiences	

Should probably define use of complimentatry pin mill work & hammer mill work.
Should have a statement why we need this supplemental work.
Should have a final statement of what we should learn by the final total body of work.

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Scale-up of batch mixing
1.1	Project / Review	Project
1.2	Technical Area	Dry Powder
2.0	Submitted by	Tim Bell,
2.1	Member company/ies	DuPont, P&G, Johnson Matthey
2.2	Idea creation date	June 23, 2015
2.3	Last modification date	June 23, 2015
3.0	Short goal description	Develop and validate a scale-up methodology for batch blending that reflects polydispersity in PSD or more than two components.
3.1	Objectives	Understand the effects of mixer scale and differences in mix component properties on scale up. Provide a framework for extension to other particle systems and mixing devices. Understand interactions between cohesive and free-flowing particles in mixing
3.2	Scope	
		Out of scope – proprietary mixer designs. Systems of free-flowing particles (only). Proposals that are exclusively computational (ie, without validation)
4.0	Contractor	Benjamin Glasser – Rutgers, Indresan Govender - Cape Town, Alessio Alexiadis - Birmingham
4.1	Comments / experiences	

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Prediction of effect of solvent and impurities / additives on crystal shape and growth kinetics
1.1	Project / Review	Project
1.2	Technical Area	Particle formation
2.0	Submitted by	Neil George / Alex Kalbasenka / Judith Bonsall / Rob Geertman
2.1	Member company/ies	Syngenta / Corbion / Unilever / DSM
2.2	Idea creation date	June 23, 2015
2.3	Last modification date	June 24, 2015
3.0	Short goal description	Develop a model of crystal growth for prediction of relative growth rate of the facets for shape prediction
3.1	Objectives	- Extend current capabilities towards prediction the effect of multi-component solvents; - Extend the model to incorporate the influence of supersaturation on the relative growth rate of different crystal facets; - Extend the model to account for impurities and additives
3.2	Scope	The model may cover the breadth of chemical functional groups including polar ones and could include impurities that could form solid solutions and adsorb on the surface such as polymers and surfactants. Prediction absolute growth face growth rates is out of scope.
4.0	Contractor	Mike Doherty, Thomas Vetter, Elias Vlieg, Matthew Neurock (Minnesota), Isabella Was…(Israel)
4.1	Comments / experiences	

IFPRI

International Fine Particle Research Institute

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Control of property distribution in particulate systems
1.1	Project / Review	
1.2	Technical Area	Systems / Measurement
2.0	Submitted by	P. Mort, A. Kalbasenka, R. Geertman, D. Braido
2.1	Member company/ies	P&G, DSM, Corbion, PSE, Horiba
2.2	Idea creation date	June 2015
2.3	Last modification date	June 22, 2015
3.0	Short goal description	1) Develop a general Population Balance Model (PBM) suitable for: a) Describing multiple particle attributes (size, shape, structure) b) Use in integrated process flow sheets (including multiple unit operations, recycles etc) c) Use in process control, including the ability to directly incorporate sensor data 2) Evaluate raw data (i.e., scattering pattern from eg laser diffraction) for use in the model (without discarding the shape and structure components of the raw data).
3.1	Objectives	Demonstrate integrated system approach to control of size distribution in particulate processes: measurement and control models 1. Determine a mathematical relationship between particle morphology and its effects on PSD measurements for technology where 2-dimensional projections of 3-D particles are used to characterize the PSD. 2. Develop a numerical model which incorporates this relationship. 3. Test the model on various particulate and measurement systems. 4. Find solutions for non-random particle orientations during analysis
3.2	Scope	Primary focus is systems modeling and measurement. The PBM model should be extended to shape and structure information in order give a description of the system state in terms of size, shape and structure of the particles. Such a model requires more sensor information than available with classic forward laser diffraction. A first

		step is to reevaluate raw data from laser diffraction to retain the shape and structure information in the output. This data should be complemented with orthogonal measurement techniques in order to get a proper deconvolution of the size, shape and structure components of the data. The deconvoluted data can then be used to feed the model.
4.0	Contractor	(Heinrich, Hamburg), A. Buch, Magdeburg, R, Nagy (Purdue), Bilgili (NJIT) …, Osaka
4.1	Comments / experiences	

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Particle Transformations during Drying
1.1	Project / Review	Project
1.2	Technical Area	Particle Formation
2.0	Submitted by	Luis Martin Rob Geertman Alex Kalbasenka
2.1	Member company/ies	DSM/Procter & Gamble/Corbion
2.2	Idea creation date	6/23/15
2.3	Last modification date	
3.0	Short goal description	Description of (pseudo) polymorphic transformations of solvated/hydrated particles during drying
3.1	Objectives	1) A kinetic description of polymorphic transformations in a dryer 2) Methods to characterize in situ the transformations in the dryer 3) Experimental validation of the model
3.2	Scope	The solvation state of particles produced during crystallization differ from the solvation state after drying. This includes changes in structure, both polymorphic transitions and formation or disappearance of amorphous material. Processes of interest are (1) solvate to anhydrous structure transformations, (2) solvate to amorphous and (3) amorphous to crystalline. Irrespective whether this is desired or undesired there is poor understanding of these transformations during drying. The transformation rate depends on the kinetics of the desolvation on a particle level and the local conditions in a dryer (p, T, RH, residence time). The work should include a description of the transformation rate depending on the process conditions on a particle scale. This description should lead to describing the circumstances in a dryer to achieve or avoid these transformations. These circumstances should be experimentally verified. Possible experimental techniques could include PXRD, Raman, FTIR, NIR, DVS. Both organic and inorganic systems can be considered. The results of the model system used should be validated against one or two industrial systems provided by IFPRI members.

4.0	Contractor	Gerard Cocquerel University Rouen Marco Mazotti ETH Zürich Lynne Taylor Purdue
4.1	Comments / experiences	