IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Filtration and deliquoring of wet cakes
1.1	Project or Review	Project
1.2	Technical Area[1]	W (yrs 1-3) / SE (yrs 4-6)
2.0	Submitted by	Gorowara, Rajeev L; Neil George; Norman Wagner; Hugh Stitt; Voort Maarschalk, Kees van der
2.1	Member company/ies	Dow, Syngenta, Johnson Matthey, Corbion
2.2	Idea creation date	14 JUN 2016
2.3	Last modification date	15 JUN 2016
3.0	Short goal description	Predict the limit of deliquoring of cakes given (predictions of) particle property distributions of dead-end filtrations optionally combined with washing
3.1	Objectives	*Basics (Wet systems context yrs 1-3)* Given particle size distribution, optionally shape distributions and wetting properties, predict: 1) Bed property evolution during dead-end filtration 2) Liquid flow patterns during deliquoring and washing of filter cake 3) Final filtration performance *Design and engineering (Systems context yrs 4-6)* Convert basic knowhow into engineering models for filtration unit operations, and: 1) Implement in flow sheet and population balance models for crystallization process 2) Recommend control approach. 3) Validation at 1-10 kg/hr scale
3.2	Scope	In scope: 1) Dead end filtrations, pressure or compression filtration, cake formation 2) Aqueous systems 3) Presence of impurities: adsorption & viscous liquids Out of scope: 1) Particle formation (particle properties given) 2) Pure water or saturated solutions (i.e. over-simplified model systems)
4.0	Contractor(s) with contact information	Basics: Karin Schroen (Wageningen University, karin.schroen@wur.nl, link)

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[1] One or more from the following list: W = wet systems; D = dry systems; F = particle formation; SR = size reduction; M = modeling; SE = systems engineering

		Filtration: Harald Anlauf (Karlsruhe Institute Technology, harald.anlauf@kit.edu, link) Systems: Thomas Vetter (Manchester University, thomas.vetter@manchester.ac.uk, link)
4.1	Comments / experiences	Collaboration project highly encouraged.

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Wetting, dispersion, disintegration, and dissolution of powders and packed beds: reconstitution of biological materials.
1.1	Project or Review	Project
1.2	Technical Area[1]	Wet Systems
2.0	Submitted by	Matt Maille, Neil George, Norm Wagner
2.1	Member company/ies	Syngenta, Guest (KGM)
2.2	Idea creation date	June 14, 2016
2.3	Last modification date	
3.0	Short goal description	
3.1	Objectives	1. Control/manipulate/engineer nano to meso scale powder surface topology and surface chemistry to promote wetting and dissolution during liquid incorporation into powder and powder beds. 2. Optimize/minimize the use of surface modifiers, such as surfactants, potential determining ions, polymers, to promote wetting and dissolution during liquid incorporation into powders in a homogeneous manner. 3. Develop and validate a mechanistic model of the particle/powder bed wetting and dissolution kinetics.
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, dispersion and dissolution. Optimal design and choice of surface modifiers will be considered with regards to powder properties. A broad range of materials are to be considered with an emphasis on water dispersible, bioderived materials of which, fully soluble particles and mixed soluble/insoluble particles are explored. Development of a phenomenological mechanistic model of the particle/powder bed wetting and dissolution kinetics will be developed and validated

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		as a predictive tool for assessing wetting/dissolution issues of material. Finally, the effects of these methods of incorporation and dispersion on rheology, including time-dependence, are to be considered.
4.0	Contractor(s) with contact information	Paul Luckham (Imperial College London), Erik Kaunisto (Chalmers University of Technology)
4.1	Comments / experiences	

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Effect of Particle Surface Properties on Particle Interactions and Bulk Powder Flow Behavior
1.1	Project or Review	Project
1.2	Technical Area[1]	Dry Systems
2.0	Submitted by	Maxx Capece, Karen Daniels, Jeremy Lechman, Jin Ooi, Antonios Zavaliangos
2.1	Member company/ies	AbbVie, Sandia National Labs
2.2	Idea creation date	14-Jun-2016
2.3	Last modification date	15-Jun-2016
3.0	Short goal description	• Identify a particle surface property and develop a methodology for the controlled modification of the property in order to alter bulk powder flow behavior. • Establish a theoretical connection between particle surface properties and bulk powder flow behavior, through application or development of mechanistic models or numerical simulations describing particle-particle interactions.
3.1	Objectives	1. Establish a method for the controlled modification of a particle surface property (leaving constant particle shape, size, or bulk material) 2. Establish a test methodology to evaluate and quantify the effect of particle surface properties on bulk powder flow behavior. 3. Develop a theoretical understanding or framework to explain the relationship between particle surface properties and bulk powder flow behavior through a mechanistic or micro-dynamic description of particle-particle interactions.
3.2	Scope	The investigation of particle surface properties (e.g. cohesion, roughness, friction, etc) on bulk powder/granular flow behavior can be carried out on any well-defined system. Surface properties should be modified in way that does not significantly alter other particle properties such as shape or size. The flow behavior should be relevant to a common industrial

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		process including but not limited to blending, screw feeding, or bin discharge. The mechanistic model or numerical simulation method used to describe particle interactions should be applied to systems that would elucidate the sensitivities or limitations of current models or simulation tools.
4.0	Contractor(s) with contact information	• Christine Hrenya (U. of Colorado) • Matthias Schroeter (Erlangen, Germany) • Rajesh Davé (NJIT)
4.1	Comments / experiences	

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IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Formation of monodisperse organic crystals
1.1	Project or Review	Project
1.2	Technical Area[1]	Formation
2.0	Submitted by	John Hone, Uli Wiesner
2.1	Member company/ies	Syngenta, Merck, …
2.2	Idea creation date	14th June 2016
2.3	Last modification date	
3.0	Short goal description	Crystallisation processes for organic molecules produce particles in the 10-150 μm range; typically requiring milling back down to the desired size. The project aim is to use a chemical or physical means (e.g. narrowly dispersed seed particles or highly porous particles) to initiate nucleation of the required number of organic crystals of the correct solid state, and then to limit the subsequent growth to the required size (including the nanoscale (<1μm)), thereby giving a narrow size distribution, and eliminating the milling step.
3.1	Objectives	1. Identify the chemical or physical means to control nucleation in organic systems so that the final particle size distribution is narrow. 2. Identify means of generating high numbers of nuclei in order to limit the final particle size. 3. Identify the chemical or physical means to stop the growth of the crystals at the required size (including sizes below 1μm).
3.2	Scope	In Scope: crystals of organic molecules Mw > 200. Narrow size distributions to minimise subsequent Ostwald ripening in the final formulation. Out of scope: inorganic systems, isolation, purification
4.0	Contractor(s) with contact information	Hitoshi Kasai (Tohoku University, Japan) Hidetoshi Oikawa (Tohoku University, Japan) Leonard MacGillivray (U of Iowa)
4.1	Comments / experiences	Emulsion crystallisations generally give large particles due to mass transport through the continuous phase. High supersaturations can produce oiling out. Some

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		metal salts of organics produce much smaller particle sizes relative to the free acid/base.

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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	Jeff Hoffmann, Paul O. Abbe Mojtaba Ghadiri, Univ. of Leeds Charles Compson, Almatis Hugh Stitt, Johnson Matthey Akihiko Ema, Nisshin Lisa Taylor, Pfizer.com Alvaro Janda, Particle-Analytics
2.1	Member company/ies	
2.2	Idea creation date	14 June 2016
2.3	Last modification date	
3.0	Short goal description	Establish empirical (i.e., not modeling) grindability for a wide range of material properties by considering the prevailing stress regime ranging from collisional to rapid shearing systems, as in hammer mills, jet mill and ball mills.
3.1	Objectives	1. Provide mechanical properties. 2. Understand material response, organic and inorganic crystalline materials. 3. Correlate materials characteristics and milling conditions.
3.2	Scope	Determination of grindability characteristics for materials with various types of mills.
4.0	Contractor	Luis Marcelo, Tavares Univ. Federal, Rio de Janeiro, Brazil Haim Kalman, Ben Gurion, Israel Stephan Heinrich, Hamburg Univ., Hamburg
4.1	Comments / experiences	

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	High-resolution surface chemical analysis of organic powders
1.1	Project / Review	Project
1.2	Technical Area	Characterization
2.0	Submitted by	Mike Gentzler, Jeff Bodycomb
2.1	Member company/ies	Merck & Horiba
2.2	Idea creation date	14-June-2016
2.3	Last modification date	14-June-2016
3.0	Short goal description	New or improved capability for chemically-specific detection and/or imaging near monolayer depth on organic powder surface.
3.1	Objectives	Create/improve & demonstrate methods for near-monolayer surface chemical heterogeneity that strongly controls powder surface energy/adhesion/forces but is currently unknown due to lack of sensitivity or destructiveness of common techniques.
3.2	Scope	Isolated biological, macromolecular, small-molecule or formulated organic powders. Surface phenomena must be (1) undetectable by common ‘surface sensitive’ solid techniques (DRIFTS, Raman) that have significant surface penetration (~ 1 um) ,and, (2) poorly discriminated by elemental techniques (like ESCA/ XPS), and, (4) compromised by standard analytical chemical techniques. Phenomena would ideally be poorly understood surface chemistry of general interest – like insulator tribocharging radicals. Contractor would be an established expert in either a specific analytical technique (e.g. SIMS or DNP-NMR) or active expert in tribocharging (or other class of) surface chemistry.
4.0	Contractor	(1) Nicholas Winograd, Penn. State, (190 SIMS pubs) (2) Bob Griffin, MIT (100 DNP pubs)* (3) Bartosz Grzybowski, UNIST, Korea (40 surface charge pubs), or Bilge & Hasan Baytekin, Bilkent Univ., Turkey (post-docs & main authors of key pubs)
4.1	Comments / experiences	*Merck collaborator

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Prediction of phase transformation from multicomponent amorphous materials
1.1	Project or Review	Project
1.2	Technical Area[1]	Particle formation
2.0	Submitted by	Justin Moser, Vincent Meunier, Paul Mort, Reinhard Kohlus
2.1	Member company/ies	Merck & Co., Inc.; Nestle
2.2	Idea creation date	14-June-2016 AGM
2.3	Last modification date	14-June-2016
3.0	Short goal description	Development of predictive models for phase stability of organic, amorphous, multi-component dispersions taking into account material properties, stresses during processing and environmental influence.
3.1	Objectives	It is proposed to focus on solid dispersions of 2 or more components that are designed to be processed into amorphous particles. Influence of material properties and processing technologies (e.g spray drying, extrusion, spray freezing/lyophilization) on quality and stability of amorphous particles should be investigated. Development of predictive models for phase stability/failure incorporating the following aspects: a. particle physico-chemical properties (e.g compositional uniformity, porosity) after processing but before aging/environmental exposure b. material properties (e.g MW, chemical structure, hygroscopicity, glass transition temperature, moisture diffusivity) c. resulting amorphous energy state/history from process stresses d. formulation or process approaches to stabilize particles (e.g coatings, moisture sinks) e. Interfacial phenomena and determination of where in the particle phase transformation (e.g nucleation) occurs

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3.2	Scope	In scope: organic, multi-component amorphous particles by design. Out of scope: inorganic materials. Products designed as a mixture of crystalline and amorphous phases.
4.0	Contractor(s) with contact information	1. Lynne Taylor – Purdue University (focus in food (Lisa Mauer) and pharma) 2. Patrick Marsac – University of Kentucky 3. Shelly J. Schmidt – University of Illinois
4.1	Comments / experiences	Lynne Taylor has an extensive history of research in this area with volumes of publications. Clearly a world expert. Patrick Marsac is a younger investigator trained under Taylor, has years of practical industrial experience and has set up a lab combining both particle processing and characterization capabilities to address this exact problem.

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	**Scale up rules for powder mixing**
1.1	Project or Review	Project
1.2	Technical Area[1]	Dry Powder
2.0	Submitted by	Michele Marigo, Prashant Gupta, Tim Bell, Marty Murtagh
2.1	Member company/ies	Johnson Matthey, P&G, DuPont, and Corning
2.2	Idea creation date	June 14, 2016
2.3	Last modification date	June 15, 2016
3.0	Short goal description	Predict how mixing mechanisms (relative importance of diffusion, convection, shear) change from bench level to production. Application to specific mixing design is open (freedom to choose mixer type or batch vs. continuous mixing).
3.1	Objectives	1. Investigating fundamental scaling rules for mixing mechanisms; 2. Predict relative importance of mixing mechanisms with mixer type & scale (length and time); 3. Determine the impact of materials properties on point 1&2;
3.2	In Scope	1. Material types (e.g. different cohesion) 2. Time scale 3. Length scale (scale of scrutiny in assessment of mixing)
	Out of Scope	1. Proprietary mixer designs. 2. Segregation systems (overly complicating) 3. Proposals that are exclusively computational (e.g. without validation)
4.0	Contractor(s) with contact information	1. Indresan Govender - UKZN South Africa 2. Benjamin Glasser – Rutgers 3. Carl Wassgren – Purdue 4. Christine Hrenya - University Colorado
4.1	Comments / experiences	1. DEM-CFD positron particle tracking for scale up of particle mixing wet and dry 2. Mixing models for scale up of particle mixing, wet and dry 3. Mixing scale up DEM 4. Particle level to bulk property continuum

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		mechanics modeling

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	**SURFACE STRUCTURAL TRANSFORMATION INDUCED BY MILLING**
1.1	Project or Review?	Project
1.2	Technical Area	Size Reduction
2.0	Submitted by	Jeff Hoffmann, Paul O. Abbe Mojtaba Ghadiri, Univ. of Leeds Charles Compson, Almatis Hugh Stitt, Johnson Matthey Akihiko Ema, Nisshin Lisa Taylor, Pfizer.com Alvaro Janda, Particle-Analytics
2.1	Member company/ies	
2.2	Date Idea creation	14-June-2016
2.3	Date -Last modification	
3.0	Short goal description	Understanding structural changes in inorganics which are or may become crystalline during size reduction.
3.1	Objectives (at least three)	Mill and evaluate materials utilizing Impact and shear type mills Wet and Dry Observing glass and other transition states Measure energetics
3.2	Scope	Measure structural changes in inorganics through various mechanisms.
4.0	Contractor (two or three)	Thomas Friscic, McGill University, Canada Mark Descamps, Univ. of Lille, France
4.1	Comments about Contractors	
5.0	Voting @ AGM	Selected / Rejected
5.1	# of Votes	