



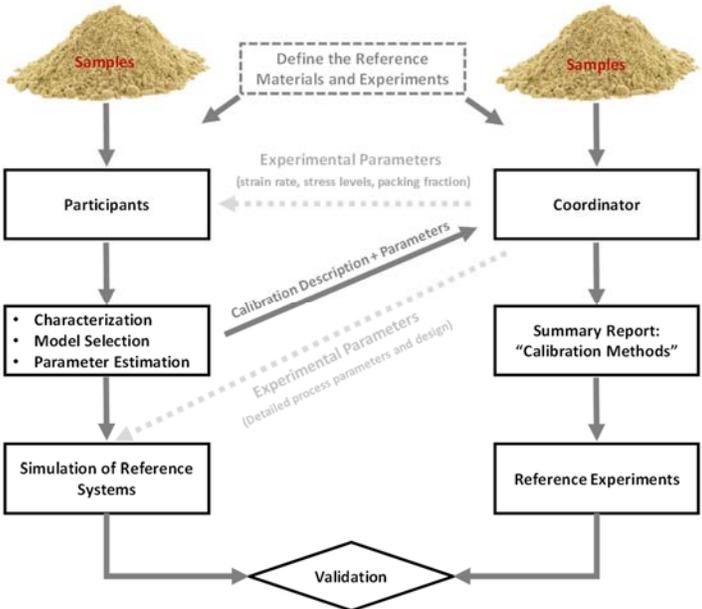
IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Round-Robin Exercise on Calibration of DEM Simulations
1.1	Project or Review	Round-Robin
1.2	Technical Area ¹	Systems Engineering / Modeling
2.0	Submitted by	Massih Pasha, Prashant Gupta, Jeremy Lechman, Emmanuela Gavi, Bill Katterhagen, David Heine, Alvaro Janda, Filip Francqui
2.1	Member company/ies	Chemours, P&G, Sandia, Roche, Pfizer, Corning, Particle Analytics, Granutools
2.2	Idea creation date	6/20/2017
2.3	Last modification date	6/21/2017
3.0	Short goal description	In the present “round-robin” exercise, an attempt will be made to examine various DEM parameter estimation/calibration methods that industrialists and academics have adopted with intention of establishing best-practices and identifying practical gaps and impediments for successful application of DEM at industrial scale.
3.1	Objectives	<p>Comparing and validating the calibration methods of DEM simulations for the quantitative prediction of flow and stress fields of both “granule” and “fine cohesive” material in “free-surface” (e.g. ‘sloped rotating drum’) and “confined” (e.g. ‘screw feeder’) systems. The calibration methods will include experimental characterization, model selection and parameter estimation.</p> <p>Cellulose microspheres (>300 μm with narrow size distribution) and reference limestone powder constitute the typical material for this study. The coordinator will review and propose the materials. Following materials are assumed to be out-of-scope:</p> <ul style="list-style-type: none"> - Material with electrostatic and/or humidity sensitivity - Material with strong adhesion to the boundaries
3.2	Scope	An academic will be contracted as the “Project Coordinator” who will be responsible for managing the project, collecting data from

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

the participants, compiling progress reports, and conducting ‘reference validation experiments’. Figure 1 shows schematically the project map for this exercise:

- Define the reference materials and experiments
- Provide reference materials to the Participants as well as the Coordinator
- Provide the Participants with “generic” info on the reference experiments
- Participants to conduct their own characterization, model selection, and parameter estimation/calibration
- Coordinator to gather description and outcome of the calibration methods used by individual participants → provide a summary report
- Coordinator to shares the details of the experimental design with the Participants
- Participants to conduct simulations of the reference systems
- Coordinator to run the reference validation experiments
- Coordinator to gathers and compares the outcomes of the modeling and experimental efforts



4.0 Contractor(s) with contact information

- Dr A Ingram (University of Birmingham, a.ingram@bham.ac.uk)
- Indresan Govender (UKZN, Govenderi5@ukzn.ac.za)
- Corné Coetzee (Stellenbosch University, ccoetzee@sun.ac.za)

4.1	Comments / experiences	<p>Timeline:</p> <ul style="list-style-type: none"> - A two-year exercise - Report of the summary of the calibration will be provided by next AGM - Summary of the validation comparison and findings will be submitted before AGM 2019 <p>Funding:</p> <table border="1" data-bbox="560 485 1398 892"> <thead> <tr> <th colspan="2" data-bbox="560 485 1292 520">Coordination & Management Activities</th> <th data-bbox="1292 485 1398 520"></th> </tr> </thead> <tbody> <tr> <td data-bbox="560 520 1292 552">Managing the program (data collection, email communications, follow-ups)</td> <td data-bbox="560 552 1292 583">Writing summary of "calibration methods and results"</td> <td data-bbox="1292 520 1398 583" rowspan="4" style="text-align: center; vertical-align: middle;">\$8.5k</td> </tr> <tr> <td data-bbox="560 583 1292 615">Writing summary of "validation and experimental results"</td> <td data-bbox="560 615 1292 646">Writing the final report</td> </tr> <tr> <td data-bbox="560 646 1292 678">The efforts equivalent to an IFPRI Review (i.e. \$8.5k)</td> <td data-bbox="560 678 1292 709"></td> </tr> <tr> <td data-bbox="560 709 1292 741"></td> <td data-bbox="560 741 1292 772"></td> </tr> <tr> <th colspan="2" data-bbox="560 772 1292 808">Validation Experiments</th> <th data-bbox="1292 772 1398 808"></th> </tr> <tr> <td data-bbox="560 808 1292 840">Distribution of samples</td> <td data-bbox="560 840 1292 871">Experimental Setup</td> <td data-bbox="1292 808 1398 871" rowspan="4" style="text-align: center; vertical-align: middle;">\$30.5k</td> </tr> <tr> <td data-bbox="560 871 1292 903">Conducting experiments</td> <td data-bbox="560 903 1292 934">Comparing participants results</td> </tr> <tr> <td data-bbox="560 934 1292 966">The efforts equivalent to 80% of one year of an IFPRI Project</td> <td data-bbox="560 966 1292 997"></td> </tr> <tr> <td data-bbox="560 997 1292 1029"></td> <td data-bbox="560 1029 1292 1060"></td> </tr> <tr> <td colspan="2" data-bbox="560 1060 1292 1092" style="text-align: right;">TOTAL</td> <td data-bbox="1292 1060 1398 1092" style="text-align: center;">\$39k</td> </tr> </tbody> </table>	Coordination & Management Activities			Managing the program (data collection, email communications, follow-ups)	Writing summary of "calibration methods and results"	\$8.5k	Writing summary of "validation and experimental results"	Writing the final report	The efforts equivalent to an IFPRI Review (i.e. \$8.5k)				Validation Experiments			Distribution of samples	Experimental Setup	\$30.5k	Conducting experiments	Comparing participants results	The efforts equivalent to 80% of one year of an IFPRI Project				TOTAL		\$39k
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Collaboration proposal between Andrew Bayly and Maarten Schutyzer.

The work of Andrew Bayly focuses on the drying at high temperatures. There is good and strong focus on the mechanical aspects of drying at high temperatures. We think that support from a scientist who is knowledgeable in material sciences, specifically (non-newtonian) rheology as function of concentration and temperature, will contribute to the scientific understanding of the project. Maarten Schutyzer from the University of Wageningen (NL) also works in the field of drying and his focus is more on the material properties. We think that a collaboration will support the IFPRI project.



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Nonlocal Rheology of Intermediate Granular Flows: Particle Shape and Size Distributions (additional collaboration)
1.1	Project or Review	Project
1.2	Technical Area ¹	Dry Flow / Characterization
2.0	Submitted by	K. Daniels, N. Vriend
2.1	Member company/ies	
2.2	Idea creation date	21-June-2017
2.3	Last modification date	
3.0	Short goal description	Extend currently-funded nonlocal rheology experiments and modeling on dry granular flows further into the intermediate flow regime, via an additional collaboration.
3.1	Objectives	The currently-funded project by this same name utilizes an apparatus which operates (1) at the low end of the intermediate flow regime and (2) on granular materials under confinement. An additional, complementary test of the nonlocal rheology could be performed by adding a second set of experiments at (1) a higher flow rate and (2) with a free boundary. A photoelastic, chute-flow apparatus is available in Nathalie Vriend's lab at Cambridge, along with the high speed camera necessary to collect the associated data on particle-trajectories and interparticle forces. Karen Daniels' lab is already collaborating with them on the photoelastic techniques required to obtain particle-scale force data (force chains) from their movies. Funds to support the collaboration would allow for the exchange of graduate students to create particles, perform additional experiments, conduct data analysis, and validate nonlocal models in this second regime.
3.2	Scope	Experimental exploration of range of flow rates and particle size distributions, extending well into the intermediate flow regime. Particle-tracking combined with photoelastic force measurements (necessitates the use of circular disks). Comparison with nonlocal rheology models.

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

		<u>Funding requested:</u> \$12k total to cover 1-2 week collaboration visits in both directions (by our respective graduate students), plus additional experimental costs associated with the new experiments, in order to make direct comparisons meaningful.
4.0	Contractor(s) with contact information	Nathalie Vriend (Cambridge) Karen Daniels (North Carolina State)
4.1	Comments / experiences	This collaboration is complementary with the McCarthy/Hill collaboration, which will quantify segregation rates in 3D intermediate flows. Having both 2D and 3D data on segregating, intermediate flows will provide important tests of the generality of the phenomena. Our groups will work together to perform these comparisons.



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Experimental Validation of Segregation Models
1.1	Project or Review	Collaboration
1.2	Technical Area	Dry Flow / Characterization
2.0	Submitted by	J. McCarthy, K. Hill
2.1	Member company/ies	
2.2	Idea creation date	21-June-2017
2.3	Last modification date	
3.0	Short goal description	Validate existing and newly developed segregation models (J. McCarthy project) in a variety of experimental flows (K. Hill lab).
3.1	Objectives	<p>We propose a collaboration between the research groups of Drs. Kimberly Hill of UMN and Joe McCarthy of U Pittsburgh to work toward experimental validation of segregation models. We will use the following experimental apparatus from Dr. Hill's lab: a split bottom cell and a long chute flow.</p> <ul style="list-style-type: none"> • The <u>chute flow</u> may be operated in both a steady and non-steady (run-out) mode, • The <u>split bottom cell</u> generates a complex, but well-characterized three dimensional flow field. <p>Comparison of experiments and operating conditions will allow a thorough test-bed for both existing and newly developed models of both density and/or size segregation. Time permitting, both groups are also interested in experimentally exploring the impact of different amounts of moisture and interparticle cohesion on the segregation rate. This collaboration is complementary with the Daniels/Vriend collaboration. Our groups will work together to perform comparisons.</p>
3.2	Scope	<p>The \$12,000 collaboration grant will cover travel of Dr. McCarthy's graduate student to UMN as well as efforts of graduate and/or undergraduate students within Dr. Hill's group. Funds are requested for:</p> <ul style="list-style-type: none"> • McCarthy (\$2,000): travel of student to UMN. • Hill (\$10,000): Support of an undergraduate researcher at UMN, associated experimental supplies, and travel for Dr. Hill to the 2018 AGM
4.0	Contractor(s) with contact information	Kimberly Hill, UMN Joseph McCarthy, Pittsburgh
4.1	Comments / experiences	



IFPRI PROJECT BRIEF TEMPLATE

1.0	(Working) Title	Effect of material properties on the adherence of powders to metal processing equipment during compaction
1.1	Project or Review	Project
1.2	Technical Area ¹	Formation (F)
2.0	Submitted by	Ketterhagen, Egan, Capece, Saurer
2.1	Member company/ies	Pfizer, Duracell, AbbVie, BMS
2.2	Idea creation date	June 20, 2017
2.3	Last modification date	June 21, 2017
3.0	Short goal description	Develop an understanding and relations between a wide range of a powder's physical/chemical properties to the undesired adhesion to metal surfaces of compaction tooling under varying process and environmental conditions.
3.1	Objectives	<ul style="list-style-type: none"> • Review and identification of relevant powder materials and a broad characterization of physical/chemical properties of said powders • Establish a test method to quantify material adhesion on compaction tooling under various process and environmental conditions • Identify key factors affecting the amount and/or rate of powder adhesion on compaction tooling due to: <ol style="list-style-type: none"> 1. molecular and crystal properties 2. substrate surface finish and chemistry 3. process conditions (e.g. pressure/stress) 4. environmental conditions (temperature, relative humidity) • Establish predictive criteria for the propensity of adherence given a set of molecular/crystal properties and process/environmental conditions
3.2	Scope	<ul style="list-style-type: none"> • Powder materials of practical industrial interest, with a wide range of mean particle sizes (e.g. ~5 um~500um)

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		<ul style="list-style-type: none"> • Process conditions including a wide range of loading stress (~50-400 MPa), temperature (e.g. 25-60 deg C), and relative humidity (e.g. 25%-75%) • To examine nominally dry, organic powders without solvent evaporation • Limited to adhesion due to mechanical stresses and/or environmental conditions • Not to include impact of formulation (e.g. lubricants) • Modeling approaches, when combined with experimental efforts, could be in scope
4.0	Contractor(s) with contact information	<p>C. Sinka (University of Leicester) +44 (0)116 252 2555 ics4@le.ac.uk</p> <p>C. Sun (University of Minnesota) 612-624-3722 sunx0053@umn.edu</p> <p>P. Tcheroloff (University of Bordeaux, France)</p>
4.1	Comments / experiences	<ul style="list-style-type: none"> • Prof. S. Beaudoin issued an IFPRI review slide pack on “Particle Adhesion to Metals” in 2016 which details theoretical aspects of adhesion of powders to metals. The relevant material properties identified in the review (e.g. Hamaker constant, DVS sorption isotherm) are expected to be included characterization approaches in this project.



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Characterization of spray drying nozzles at industrially-relevant conditions
1.1	Project or Review	Project
1.2	Technical Area	Formation
2.0	Submitted by	Christine Colby, Poul Bach, Joe Bullard, Justin Moser
2.1	Member company/ies	Aveka, Novozymes, Vertex Pharmaceuticals, Merck
2.2	Idea creation date	20-06-2017
2.3	Last modification date	21-06-2017
3.0	Short goal description	<p>The approach to spray drying varies broadly by industrial application, using several different spray nozzle types and a wide range of operating parameters (mass flow, velocity and pressure), spraying fluids with myriad rheological properties in different chamber conditions (temperature and pressure). Although, there is a large body of literature on spray characteristics, little is focused on comparing sprays at conditions relevant to spray drying industry. The purpose of this research is to map the breadth of spray characteristics for a broad range of industrially relevant fluid systems and operating conditions to enable the selection of a set of nozzles and conditions for a given application. The best choice of nozzle for an application depends in most cases strongly on specifics of the application. It may be critical to limit oversize particles in some application or undersize particles in other. Just focusing on an average particle size, as most of the current correlations do, is rarely sufficient.</p>
3.1	Objectives	<ul style="list-style-type: none"> - Determine droplet size distributions for a range of flow parameters at different distances from the nozzle. - Develop a comparison map of different nozzles identifying their operating range and limitations in terms of the quality of the atomization, defined in terms of size distribution, droplet shape distribution, stability and fluctuation of the spray.
3.2	Scope	<p>In order to limit the range of parameters, it is suggested to characterize sprays at the following conditions:</p> <p>(1) Two different nozzle types with three different scales: (a) Twin-fluid nozzle: 3 small scale nozzles used by the industry; (b) pressure swirl nozzle: 3 small nozzles used by the industry.</p> <p>(2) Several different fluid types with varying viscosities: Water-Glycerin mixtures, water-maltodextrin solutions, complex fluid with varying shear and extensional viscosities, fluid with suspensions (e.g. clay, kaolin..), organic polymer solution (Pharmaceuticals), and/or member company suggestions (with supplied materials).</p> <p>(3) Different chamber temperatures.</p>
4.0	Contractor(s) with contact information	<p>(1) Nasser Ashgriz, Uni. Of Toronto. ashgriz@mie.utoronto.ca (2) B. Mulhem University of Bremen, Chemical Engineering Department, mulhem@iwt.uni-bremen.de</p>
4.1	Comments / experiences	



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	cohesion United
1.1	Project or Review	Project
1.2	Technical Area ¹	Dry systems
2.0	Submitted by	Tim Bell, Tim Freeman, Michel Louge, Jeremy Lechman, Massih Pasha, Paul Mort
2.1	Member company/ies	DuPont, Freeman Tech, Sandia National Labs, Chemours, P&G
2.2	Idea creation date	June 20, 2017
2.3	Last modification date	
3.0	Short goal description	Establish the role of cohesion on powder flow
3.1	Objectives	<ol style="list-style-type: none"> 1. Establish a method for the controlled modification of particle cohesion. 2. Characterize cohesion at the particle scale, as well as at the scale of bulk characterization instruments. 3. Establish the role of cohesion on a dynamic flow of industrial interest, such as a hopper, a chute, a blender, or a screw feeder.
3.2	Scope	Consistent with recommendations from most participants of the January 2017 Powder Flow Workshop (hence the adjective “United” in the title), cohesion will be characterized at the particle and bulk levels, and its effect on a dynamic flow will be established and modeled.
4.0	Contractor(s) with contact information	<p>Joshua Dijkstra, https://www.wur.nl/en/Persons/dr.-JA-Joshua-Dijkstra.htm</p> <p>Christine Hrenya (U. of Colorado) http://www.colorado.edu/chbe/christine-m-hrenya</p> <p>Matthias Schroeter (Erlangen, Germany) http://www.mss.cbi.fau.de/people/single/schroeter-dr-rer-nat-habil-matthias</p>
4.1	Comments / experiences	

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IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Flow at boundaries – spreading particles in thin and uniform layers
1.1	Project or Review	Project
1.2	Technical Area ¹	Dry Flow / Characterization
2.0	Submitted by	M. Louge, P. Mort, F. Francqui, Vidyapati, D. Bolintineanu, T. Bell, T. Freeman
2.1	Member company/ies	Granutools, DuPont, P&G, Sandia, Freeman
2.2	Idea creation date	20-June-2017
2.3	Last modification date	21-June-2017 (v2, PRM, FF, VV, DB)
3.0	Short goal description	Develop extensions for dry-flow rheology describing flow, stress, and packing density at boundaries including a free surface. Include industrially-relevant powder flow characterization techniques relevant to flows at boundaries.
3.1	Objectives	<p>Characterize and predict flows relevant to thin layers of particles, where layer thickness (H) is no more than 10X the median particle size (D), spread over a width (W) that is relatively large: $H/D < 10$; $W/H > 100$.</p> <p>The flux of layer deposition should include quasi-static and dense intermediate flow regimes, where the flow regime is defined at the point of metering flow into the layer.</p> <p>Define functional relationship between particle characteristics, relevant powder characterization techniques, and process characteristics (achievable deposition flux, layer flatness, local packing density, deposition RSD).</p>
3.2	Scope and Context	The flow of powders under low consolidation stress and with a free surface is relevant to a range of industrial processes and emerging technologies. Conditions of low consolidation stress are encountered in many applications: fluidized bed, small silos, capsule filling, additive manufacturing, etc. In these applications, cohesion may induce flow intermittences, waves and complex density fluctuations [1]. These phenomena are relevant in processing, for example in powder-bed-based

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		<p>additive manufacturing where the creation of successive thin and homogenous powder layer is needed [2].</p> <p>In order to select the best powder properties and to optimize the process, we need modeling and characterization methods relevant to flows that are dominated by boundary-layer physics. Ideally, measurement methods should reflect the flow, stress and packing fields of powders in thin-layer flows.</p> <p>Validation should include a practical range of boundary conditions on the thin-layer substrate (e.g., previous free surface, belt, etc.) and underflow boundary (e.g., weir or roller) used to control layer thickness. Experimental and computational techniques should be able to capture a range of particle size, shape and density distribution, as well as variations in bulk cohesion and particle mechanical properties (e.g. modulus, roughness).</p> <p>[1] M. Wojtkowski, O. I. Imole, M. Ramaioli, E. Chávez Montes and S. Luding, Behavior of cohesive powder in rotating drums, AIP Conference Proceedings 1542 (2013) [2] G. Yablokova, M. Speirs, J. Van Humbeeck, J.-P. Kruth, J. Schrooten, R. Cloots, F. Boschini, G. Lumay, J. Luyten, Rheological behavior of β-Ti and NiTi powders produced by atomization for SLM production of open porous orthopedic implants, Powder Technology 283, 199–209 (2015)</p>
4.0	Contractor(s) with contact information	Steve Morris (Toronto) Nicholas Taberlet (Lyon) C Fred Higgs (Carnegie Mellon) MAPP (Manufacturing using Advanced Powder Process) led by University of Sheffield
4.1	Comments / experiences	



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Modeling of Twin Screw Feeders for Continuous Manufacturing
1.1	Project or Review	Project
1.2	Technical Area ¹	Systems Engineering (SE)
2.0	Submitted by	Justin Moser, Sean Bermingham, Bill Ketterhagen
2.1	Member company/ies	Merck, PSE, Pfizer
2.2	Idea creation date	20-Jun-2017
2.3	Last modification date	20-Jun-2017
3.0	Short goal description	<ul style="list-style-type: none"> In order to reduce the significant amounts of material currently used to experimentally characterize feeders, it is necessary to develop an improved twin screw feeder model that incorporates effects of varying input material properties (incl. cohesion) and equipment properties for control of flow rate as $f(\text{time})$. Combination of multiple instances of this predictive model (for feeding different powders) plus RTD blender models will enable prediction of variability in final product composition.
3.1	Objectives (general chronological order)	<ul style="list-style-type: none"> Review and identification of the target feed material properties and equipment parameters and experimental means of measurement (both for small scale material characterization used to provide inputs to feeder model as well as data from feeder trials for model verification). Identification of appropriate models for interrogation for the problem at hand. This includes precise definition of the input variables and desired responses to model. In addition, the physics involved that need to be accounted for (e.g. multiphase flow from entrapped air, particle friction). Mechanistic models are favored but it may be necessary to introduce a data driven element to capture the high frequency fluctuations in feeder flow rate. Development of an appropriate feeder model to handle a wide range of material properties, equipment parameters and boundary conditions <ul style="list-style-type: none"> Inputs for consideration: Equipment geometry (screw geometry & scale, hopper design), Product (PSD, shape, internal friction/cohesion, compressibility), Process (screw speed, hopper level, boundary conditions (e.g. free fall vs back pressure gradient)) Responses: Screw fill %, RTD, flood feeding limit, granular temperature, particle collisions and corresponding friction, feed factor (g/rev), mass flow rate, flow rate variability as $f(\text{time}, \text{feed rate})$ Calibration and validation of the model using real example(s) of industrial powders/granules. Comparison of model output vs experimental measurement of said powders/granules. Project should be an appropriate balance of experimentation (small scale

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		for material characterization and large scale to validate model-based methodology) and modeling.
3.2	Scope	<ul style="list-style-type: none"> • Powder and granular materials of practical industrial interest. Size (e.g. 5-1000 microns), elasticity, compressibility, varying shapes and cohesion. • Twin screw feeders for said powder and granular materials. • All relevant material properties including size, shape, cohesion (particle level friction), compressibility, density. • All models that serve the objectives of the project. These likely could include mechanistic models and hybrid mechanistic-statistical models. Preferably keeping DEM approaches limited or out of scope.
4.0	Contractor(s) with contact information	<ol style="list-style-type: none"> 1. Aibing Yu Professor Dept. of Chemical Engineering Email: Aibing.Yu@monash.edu Phone: +61 3 99050582 2. Johannes G. Khinast Institute for Process Engineering Pharmaceutical and Process Engineering Graz University of Technology AUSTRIA Tel: (0316) 873 7978 Email: khinast@tugraz.at 3. Carl Wassgren Professor of Mechanical Engineering and Industrial and Physical Pharmacy (by courtesy) School of Mechanical Engineering 585 Purdue Mall Purdue University West Lafayette, IN 47907-2088 U.S.A. Office: ME 3003J E-mail: wassgren@purdue.edu
4.1	Comments / experiences	



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Multi-scale modelling of spray drying processes
1.1	Project or Review	Project
1.2	Technical Area ¹	Systems Engineering, Particle Formation
2.0	Submitted by	Pavithra Sundararajan, Sean Bermingham, Christine Colby, Emmanuela Gavi
2.1	Member company/ies	Merck, PSE, Aveka, Roche (Potential area of interest to Keurig, Milk Specialties, Nestle, Novozymes, P&G, Pfizer)
2.2	Idea creation date	20 June 2017 AGM
2.3	Last modification date	21 June 2017
3.0	Short goal description	Prediction of particle properties arising from a spray drying process taking into account thermodynamics of multi-component solvents and solute, fluid and particle dynamics and overall process flowsheet configuration and operation.
3.1	Objectives	<p>Demonstrating the ability and value of combining multiple systems dimensions:</p> <ol style="list-style-type: none"> 1. Multiple length scale models: coupling thermodynamics, particle and fluid dynamics (Eulerian-Lagrangian CFD), droplet scale models in the dryer with population balance based unit operation models for compressor, condenser, cyclone and baghouse. 2. Global sensitivity analyses to identify regions of robust operation of the dryer providing particles in the desired attribute range. <ol style="list-style-type: none"> a. Evaluating the transience in the operation due to disturbances introduced in the system to understand the model's ability to predict system failure (or robustness). b. Study differences between different dryers and sizes to understand the ability to transfer a spray drying process between scales seamlessly.
3.2	Scope	<p>Proposed approach:</p> <ol style="list-style-type: none"> 1. Flowsheet modelling: Combining the multi-scale spray dryer model with unit operation models for the compressor, condenser, cyclones and baghouse operating in a closed loop. The flowsheet modelling is required to ensure the spray dryer is fed with the

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		<p>correct information of the recycled drying gas.</p> <ol style="list-style-type: none"> 2. This would couple the systems level model by accounting for thermodynamics exchange and flow through all its components, while iteratively interfacing with a multi-scale CFD model of drying chamber for residence time prediction as a function of particle size. 3. Calibration (heat loss, nozzle – droplets, etc) and validation of the multiscale model to selected spray dryers (small and large scale), and model solution systems.
4.0	Contractor(s) with contact information	<p>Markus Kraft, University of Cambridge https://como.cheng.cam.ac.uk/index.php?Page=Research (top of the list because his group is a computational modeling group that focuses on building flow sheet models but also has a lot of experience in CFD modeling. Handscomb’s work came from this lab) E. Tsotsas (CFD expertise) http://www.ovgu.de/ivt/tvt/index.php?idcatside=55&lang=2 R. Vehring, U. Alberta https://sites.ualberta.ca/~vehring/PE%20Page/Research.html</p>
4.1	Comments / experiences	



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Investigation of particle characteristics on high solids rheology
1.1	Project or Review	Project
1.2	Technical Area ¹	Wet systems
2.0	Submitted by	Marty Murtagh, Wilson Poone, Hugh Stitt, John Horn
2.1	Member company/ies	Corning, US Army, Arkema, JM, Sandia, Syngenta, Chemours, P&G
2.2	Idea creation date	June 20, 2017
2.3	Last modification date	
3.0	Short goal description	Explore the link between the packing and rheology of concentrated suspensions, e.g., by varying particle morphology, inter-particle friction and size distribution.
3.1	Objectives	Understand the impact of pre-processing and feed materials on suspension flow
3.2	Scope	Monitor structure and dynamics under flow; develop framework linking measured structure and dynamics to constitutive properties of suspension; develop toolkit for systematic variation of relevant parameters
4.0	Contractor(s) with contact information	Daniel Blair (Georgetown) e: dlb76@georgetown.edu Daniela Kraft (Leiden Institute of Physics, Netherland) e: kraft@physics.leidenuniv.nl Erin Koos (KU Leuven, Belgium) e: erin.koos@kit.edu
4.1	Comments /experiences	Daniel Blair: Research interest; confocal microscopy and rheology (bulk and micro) to investigate the micromechanical structure and properties of soft glassy solids Daniela Kraft: Research interest; physics and self-organization of soft matter systems. Including the rational design of anisotropic and patchy particles for use as model systems and self-assembly Erin Koos: Scholar at KIT Karlsruhe and came from Caltech granular mechanics group for her PhD. Research interest: Investigating two-fluid “capillary” suspensions in detail describing both their underlying physical structures and the influence on the rheology concentrating on the structural changes made by the solid fraction, contact angle, and external forces. Evaluation of initial applications.

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



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Predicting & characterizing surface modification during milling
1.1	Project or Review	Project
1.2	Technical Area ¹	Size Reduction
2.0	Submitted by	Rajeev Gorowara, Dupont Mike Gentzler, Merck Chuck Compson, Almatris Lisa Taylor, Pfizer Hubert Mueller, Evonik Christophe Grosjean, Syngenta Vincent Meunier, Nestle Massih Pasha, Chemours
2.1	Member company/ies	Dupont, Merck, Almatris, Pfizer, Evonik, Syngenta, Nestle , Chemours
2.2	Idea creation date	6/20/2017
2.3	Last modification date	6/21/2017
3.0	Short goal description	Predict/simulate and later characterize physical/mechanical properties of crystals and chemical/physical (-surface) transformation in a crystal in response to shock impact by atomic/molecular level simulation as would occur in milling processes. - Experimentally validate with collaboration project. Experimentally validate to extent possible.
3.1	Objectives	The motivation is to help bridge understanding between-of surface structure changes and-during production milling. Size reduction is often a final processing step to achieve desired PSD, however the final particles often show undesirable surface changes that are difficult to predict. (1) Computational prediction of physical surface transformations, specifically focused on molecular level change that underlies plasticity within semi-brittle breakage. Examples could be localized phase transformation (new form or amorphization), plastic strain

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Commented [MG1]: I do not think the current state of modelling capability is such that prediction would be possible. I think it is more realistic to say: "Explore the link between the two"!

Also I think organic and inorganic crystal transformations are completely two different kettle of fish, and mixing them could disappoint both parties!

Commented [MG2]: I think we should be realistic here. Modelling of crack propagation and its prediction from an atomistic/molecular base is not established yet!

The best reference for Quasi-continuum simulations of fracture and crack propagation is the community website qcmethod.org. This page lists a selection of related references.
<http://qcmethod.org/publications>

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

		<p>to the existing crystal, defect formation, fracture planes...etc... that occur as a result of impact rates as would occur in standard mills (ball mills, jet mills, hammer mills, attrition mills).</p> <p><u>(2) Prediction of equilibrium crystal mechanical / phase response would be a preliminary step.</u></p> <p><u>(3) Further effort beyond year 3 could incorporate chemical transformation in the simulation if appropriate.</u></p> <p><u>(4)</u></p> <p>Experimental systems selection and validation by <u>characterization techniques</u> needs to be proposed, likely in conjunction with a collaborator.</p>
3.2	Scope	<p>Crystalline <u>solid materials</u> (inorganic or organic, or both)</p> <p>Semi-brittle</p> <p>Single crystal (<u>MD methods include different orientations</u>) or polycrystalline (<u>quasi-continuum methods</u>)</p>
4.0	Contractor(s) with contact information	<p><u>M. Ortiz, Dept. Aeronautics, Caltech</u></p> <p><u>Doros Theodorou, Sch. Chem Eng., National U. of Athens</u></p> <p><u>W.K. Liu, Dept. of Mechanical Eng., Northwestern</u></p> <p>Sally Price, University College London</p> <p><u>Doros Theodorou, Sch. Chem Eng., National U. of Athens</u></p> <p><u>W.K. Liu, Dept. of Mechanical Eng., Northwestern</u></p>
4.1	Comments / experiences	<p><u>Should-Could</u> be a collaborative project starting with computation and adding an experimentalist. Potential list of collaborators:</p> <p>Mervyn Miles, University of Bristol</p> <p>Hartwig Steckel, Christian Albrecht, U. of Kiel</p> <p>Marc Descamps, Univ. of Lille</p> <p>Clive Roberts, Univ. of Nottingham</p> <p>Ken Morris, Long Island Univ.</p> <p>Steve Beaudoin, Purdue</p>

Commented [MG3]: I recommend to go for a physicist rather than a pharmaceutical technologist, as the latter tends to be pragmatist and tends to empiricism, due to the very wide range of crystalline structure behavior in organic solid state!

Commented [MG4]: As above!



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Wetting, dispersion, disintegration, and dissolution of powders and packed beds: reconstitution of organic/biological materials.
1.1	Project or Review	Project
1.2	Technical Area ¹	Wet Systems
2.0	Submitted by	Matt Maille, Judith Bonsall, Vincent Meunier, Norm Wagner
2.1	Member companies	Keurig Green Mountain, Unilever, Nestle
2.2	Idea creation date	June 20, 2017
2.3	Last modification date	
3.0	Short goal description	
3.1	Objectives	<ol style="list-style-type: none"> 1. Control/design/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/powder beds in a homogeneous manner. 3. Develop and validate a mechanistic model of the particle/powder bed wetting and dissolution kinetics.
3.2	Scope	<p>Imbibition and dispersion of organic/bio 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, imbibition, and dispersion. Additives such as surfactants, ions, and polymers as well as combinations thereof, are often used to promote imbibition, dispersion and dissolution. Optimal design of surface properties and particle morphologies will be considered with regards to powder reconstitution. A focus on food/pharma materials, with an emphasis on water dispersible, bioderived materials of which, fully soluble particles and mixed soluble/insoluble particles are explored. A phenomenological mechanistic model of the particle/powder bed wetting and dissolution</p>

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

		kinetics will be developed and validated as a predictive tool for assessing wetting/dissolution issues of powders/powder beds in both confined and unconfined vessels. Finally, the effects of these approaches of changing imbibition and dispersion, with regards to time-dependence, are to be considered.
4.0	Contractor(s) with contact information	Paul Luckham (Imperial College London), [Primary] Erik Kaunisto (Chalmers University of Technology) [Primary] Francois Lequeux (ESPCI Paris) [Secondary]
4.1	Comments / experiences	

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Methods (experimental and numerical) for describing wall boundary layer in high shear systems (Extruders or similar systems)
1.1	Project / Review	Review
1.2	Technical Area	Characterization & modelling, wet system
2.0	Submitted by	Michele Marigo (JM), Jonathan Oliver (JM), Judith Bonsall(Unilever) Patrick McGuire (Unilever)
2.1	Member company/ies	JM, Unilever, & Corning
2.2	Idea creation date	June 2017
2.3	Last modification date	
3.0	Short goal description	<p>Wall slip is a fundamental component to the way that high solid dispersions respond to mechanical deformation.</p> <p>The goal is to evaluate experimental methods and modelling approaches to describe high shear flow at wall boundaries for multiphase systems: from granular to wet system from medium to high solid content specifically when undergoing processes such as extrusion, injection molding, .</p>
3.1	Objectives	To identify state of the art and current practices for both experimental methods and modelling approaches
3.2	Scope	<p>Approaches to investigate wall boundary layer for high shear systems</p> <p>Approaches to model wall boundary layer for high shear systems</p> <p>Methods to investigate mechanisms leading to wall effect (e.slip, stick flow) at high shear including but not exclusively: thermal, material surfaces and ect.</p> <p>Experimental approaches/methods for testing</p> <p>Modelling to characterization techniques and results</p> <p>Dry to comparatively medium- high solids content materials (not only on polymers)</p>
4.0	Contractor	<p>Mike Adams (University of Birmingham), Eric Windhab (ETH), Germany Franhoufer(?)...Michel Cloitre - ESPCI Paris [Soft Matter & Chemistry Group]</p> <p>https://www.mmc.espci.fr/spip.php?article27</p> <p>Bonnecaze, Roger T - University of Texas at Austin</p> <p>http://che.utexas.edu/faculty-staff/faculty-directory/bonnecaze-2/</p>
4.1	Comments / experiences	Experimental and modelling approaches
5.0	Voting @ AGM	Selected / Rejected
5.1	# of Votes	
6.0	Contractor preference	Rank the contractors

IFPRI PROJECT / REVIEW BRIEF TEMPLATE

		1. (who / #votes) 2. (who / #votes) 3. (who / #votes)
6.1	Progress in contacting	Date contacted #1 Acceptance / Rejection (Date) Date contacted #2 Acceptance / Rejection (Date) Date contacted #3 Acceptance / Rejection (Date)



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	On-line prediction of bulk density of powder beds from starting powder particle size and shape distribution
1.1	Project or Review	Review
1.2	Technical Area ¹	Characterization
2.0	Submitted by	Navin Venugopal, Bill Schwerin, Rick Cook
2.1	Member company/ies	Corning, Honeywell-UOP, Energizer
2.2	Idea creation date	6/20/2017
2.3	Last modification date	6/20/2017
3.0	Short goal description	Understand the impact of particle physical properties, such as shape distribution and size distribution on the bulk assembly and density on-line and/or in-line during powder conveyance to provide real-time feedback in industrial processes
3.1	Objectives	-Survey of state of the art for models of continuous particle size distribution and/or irregular shape systems and packing effects -Modeling cohesivity/flowability and the the influence (and/or confounding) of particle packing models
3.2	Scope	-Dry powder systems -DEM simulation of two systems of extreme difference
4.0	Contractor(s) with contact information	<ol style="list-style-type: none"> 1. Eric J.R. Parteli, Friedrich-Alexander-Universität Erlangen-Nürnberg (Germany) 2. Ali Hassanpour, University of Leeds (UK) 3. Miguel Ángel Martín, Department of Applied Mathematics, E.T.S.I. Agrónomos, Universidad Politécnica de Madrid, Madrid (Spain) 4. Salvatore Torquato, Princeton University (US)
4.1	Comments / experiences	

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



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Measurement techniques at the particle level to map the spatial location of Minor Components present within engineered particles
1.1	Project or Review	Review
1.2	Technical Area ¹	Characterization Sub Group
2.0	Submitted by	Chris Rueb – AVEKA Rick Cook - Energizer
2.1	Member company/ies	many
2.2	Idea creation date	6/20/17
2.3	Last modification date	6/20/17
3.0	Short goal description	Review the numerous intrusive and unintrusive analytical techniques to measure and map the special location and distribution of minor components within engineered particles.
3.1	Objectives	Review paper Identification of old and new emerging techniques used.
3.2	Scope	Minor Components are defined as amount of materials at 10vol% or less including as low as ppm levels. Minor components may be things like highly valuable pharma actives, nutraceuticals, enzymes, fragrance oil droplets, and pesticides, catalysts in an agglomerate or microcapsule. Minor components may also be necessary but not always desired additives, adjuvants, and binders in an agglomerate or microcapsule. Minor components that are Organic or Inorganic are in scope. Engineered particles from 10 microns – 1000 microns are in scope. Engineered particles holding the minor components may be individual particles like microcapsules, or agglomerates.
4.0	Contractor(s) with contact information	Krister Holmberg Professor; Chemistry and Chemical Engineering, Applied Surface Chemistry krister.holmberg@chalmers.se ☎ +46 31 772 29 69

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

		option 2: Prof Zhang – University of Birmingham
4.1	Comments / experiences	It is common to include or be forced to have minor components present in an engineered particle. The ability to spatially determine the location and distribution of these minor components will help in the future design and manipulation of such particles. This information also will help all industries in developing engineered particles through process and materials choices. There are certainly many established and emerging analytical techniques used to evaluate the distribution of these minor components which can be learned from this review.



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Functional Encapsulation
1.1	Project or Review	Review
1.2	Technical Area ¹	Formation
2.0	Submitted by	Kees Maarschalk and Jim Litster
2.1	Member company/ies	Corbion
2.2	Idea creation date	20/06/17
2.3	Last modification date	20/06/17
3.0	Short goal description	A review of the techniques for functional encapsulation. Many products from many industry sectors are coated to functionalise the particle or to protect the functionality of the particle. A wide variety of techniques is used. This will be a critical review focusing on functionalities and performance on the one hand and coating formulations and encapsulation technologies on the other hand. Ideally, this review is the basis of for encapsulation technology selection for a given challenge.
3.1	Objectives	<ol style="list-style-type: none"> 1. State of the art of available techniques for encapsulation and particle coating; 2. Review of encapsulation materials available in relation to encapsulation techniques; 3. Critical review of advantages and disadvantages, scope and limitations, of different techniques.
3.2	Scope	In scope: encapsulation, particle coating Out of scope: surface functionalization
4.0	Contractor(s) with contact information	Cordelia Selomulya (Monash)
4.1	Comments / experiences	

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



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Use of grinding aids in dry systems (organic/inorganic)
1.1	Project or Review	Review
1.2	Technical Area ¹	Size Reduction
2.0	Submitted by	C. Compson, Almatis W. Hendrickson, AVEKA J. Hart & N. Treat, Imerys G. Davis, Duracell
2.1	Member company/ies	Almatis AVEKA Duracell
2.2	Idea creation date	6/20/2017
2.3	Last modification date	
3.0	Short goal description	Review the use of grinding aids in dry milling of organic and inorganic materials
3.1	Objectives	What is/are the purposes of grinding aids? What is the mechanism by which they work? What is impact on energy & comminution efficiency? What types of mills are applicable? What is the change in surface chemistry?
3.2	Scope	Dry systems/dry grinding Dry or liquid grinding aids Inorganic materials Organic materials Positive or negative effects of aids Include water, steam
4.0	Contractor(s) with contact information	Heekyn Choi, Chnagwan Nat. Univ., South Korea P. Somasandran, Columbia Univ., New York Robert Flatt, ETH, Zurich, Swiss Arno Kwade, U. of Braunschweig, Germany
4.1	Comments / experiences	

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



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Relative Humidity and the Flowability of Hygroscopic powders and granules
1.1	Project or Review	Review
1.2	Technical Area ¹	Characterization
2.0	Submitted by	Lee Hagre, Keith Swain,
2.1	Member company/ies	Horiba, IFP, Inc.
2.2	Idea creation date	20-Jun-2017
2.3	Last modification date	20-Jun-2017
3.0	Short goal description	Review of parameters and test methods to understand the effects of relative humidity on the flow characteristics of hygroscopic particles and granules
3.1	Objectives	Provide quantification of the critical parameters that influence the flowability of hygroscopic powders and granules in a manufacturing environment.
3.2	Scope	In-scope: Manufactured powders known to be effected by atmospheric moisture used in industrial manufacturing processes. Should include industries of food, pharmaceutical, and industrial materials
4.0	Contractor(s) with contact information	<ol style="list-style-type: none"> 1. Geoffroy Lumay, APTTIS, University of Liege, Belgium Geoffroy.lumay@ulg.ac.be 2. Uli Wiesner, Cornell University
4.1	Comments / experiences	<ol style="list-style-type: none"> 1. Author of publication in Journal of Drug Delivery Science and Technology “Effect of relative humidity on the flowability of lactose powders” 2. Cornell has an advanced food science research program.

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



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Review of theoretical and experimental study of initial state of solids incorporation into liquids
1.1	Project or Review	Review
1.2	Technical Area ¹	Wet Systems
2.0	Submitted by	Vidyapati (Vidya)
2.1	Member company/ies	P&G.
2.2	Idea creation date	
2.3	Last modification date	
3.0	Short goal description	Many industrial processes involve incorporation of dry powders into liquids. The entire transformation consists of many steps like impinging the liquid interface, wetting, dispersion and suspension/sediments. In some cases solids can undergo hydration, erosion and dissolution. The initial state of contact between solids and liquid determines the subsequent transformations. There are many factors affecting initial distribution of solids at the liquid interface, these may include, the powder feed rate, particle-particle interaction at dry state, powder physical properties, powder liquid interaction, and hydrodynamic condition of liquid.
3.1	Objectives	We would like to propose a review of previous work, experimental as well as theoretical in the field of powder dispersion focusing on distribution of aggregate/discrete particles at the liquid surface.
3.2	Scope	Powder of primary particles from 20-500 microns. We are interested in solids loading of 1 to 20%. Powder feed rate could be steady as well as transient.
4.0	Contractor(s) with contact information	Prof. Don Feke, Case Western University; Henk G Merkus, Delft University; Wilson Poon, University of Edinburgh Gul Oscan-Taskin, who is now at Loughborough University N.Ozcan-Taskin@lboro.ac.uk

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

		She worked many years in the industry as a consultant and led an industrial consortium on the topic (http://www.lboro.ac.uk/departments/chemical/about/people/gul-ozcan-taskin/)
4.1	Comments / experiences	



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Melt crystallization control of polymers, lipids and formulations, control of lag time
1.1	Project or Review	Review
1.2	Technical Area ¹	Formation
2.0	Submitted by	Kees Maarschalk, Dan Brady, Uli Wiesner
2.1	Member company/ies	Corbion, PSE
2.2	Idea creation date	20 JUN 2017
2.3	Last modification date	
3.0	Short goal description	Many particle formation processes using melts see that there is a lag-time between particle formation and crystallization. This implies many different issues related to process and product performance control. Examples are handling the not-yet crystallized particles and large variations in product attributes. Examples of materials exhibiting this behavior are molten polymers, lipids and their formulations. The goal of this review is to survey the current level of understanding of the kinetics of crystallization from melts of relatively large molecules.
3.1	Objectives	A review describing ... <ol style="list-style-type: none"> 1) the mechanisms of crystallization from melts, 2) with specific emphasis on polymers, lipids and formulations thereof. 3) Specific emphasis should be given to kinetics of crystallization (nucleation and growth) and... 4) the effects of foreign compounds such as impurities
3.2	Scope	In: <ul style="list-style-type: none"> - melts of polymers and lipids - formulations thereof - impurities - kinetics of crystallization, influencing factors Out: <ul style="list-style-type: none"> - proteins and other biomolecules - solutions
4.0	Contractor(s) with contact information	Thomas Thurn Albrecht (University Halle-Wittenberg, thomas.thurn-albrecht@physik.uni-halle.de)

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

		Francesco Picchioni (Groningen University f.picchioni@rug.nl)
4.1	Comments / experiences	



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Taxonomic review of powder flow
1.1	Project or Review	Review
1.2	Technical Area ¹	Dry systems
2.0	Submitted by	Michel Louge, Tim Freeman, Paul Mort, Tim Bell
2.1	Member company/ies	Freeman Tech., P&G, DuPont
2.2	Idea creation date	June 20, 2017
2.3	Last modification date	
3.0	Short goal description	Classify powder flows with respect to particle properties, boundary conditions and process stress / strain regimes
3.1	Objectives	<ol style="list-style-type: none"> 1. Review flows used in industrial applications. 2. Determine a taxonomy of flows distinguishing boundary conditions, particle properties and confinement.
3.2	Scope	<p>Unlike the GdR Midi review article https://arxiv.org/pdf/cond-mat/0312502.pdf, recognize that granular rheology is not determined solely by the bulk in an all-encompassing rheological correlation, but instead is crucially influenced by the nature of boundaries. The reviewer will come up with a taxonomy that will distinguish cohesive vs non-cohesive particles; confined vs unconfined; side walls present or not; free surface vs interior flows, quasi-static vs dynamic, etc.</p>
4.0	Contractor(s) with contact information	<p>Renaud Delannay, U. Rennes, https://ipr.univ-rennes1.fr/d5?mtop=dpt5&lang=en Nicolas Taberlet http://perso.ens-lyon.fr/nicolas.taberlet/ Alexandre Valance https://ipr.univ-rennes1.fr/membre?display_who=111&lang=en Khaysher Saleh, University of Compiegne, France</p>
4.1	Comments / experiences	

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



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Review of Multiphase/Multiscale Modelling and Simulation Methods of Particle Technology Applications
1.1	Project or Review	Review
1.2	Technical Area ¹	Systems
2.0	Submitted by	James Michaels and Jeremy Lechman
2.1	Member company/ies	IFPRI, Sandia Labs
2.2	Idea creation date	June 17, 2017
2.3	Last modification date	June 20, 2017
3.0	Short goal description	Fundamental questions in particulate materials applications (design, formation, processing and materials) are often intertwined with the complexities of multiphase and multicomponent systems. Relevant phenomena span multiple scales and are sensitive to coupling of the physical processes of mass, momentum and energy transport which are often nonlinear and nonequilibrium. This complexity makes it increasingly clear that modeling and simulation has a crucial role to play in elucidating the physical mechanisms and quantitative details leading to increased prediction and control of manufacturing processes. To wit, a review of state-of-the-art numerical modeling and simulations approaches to multiphase and multiscale numerical modeling and simulation is requested. The review should address a broad range of methods, their physical assumptions, mathematical description, numerical/computational/algorithmic practicalities and the challenges of applying them to problems of industrial relevance to particulate technology.
3.1	Objectives	Survey and summarize potential numerical methods of consequence to industrial applications related to particle technology (design, formation, processing, materials, and performance). Provide good introduction to physical basis, mathematical description, and numerical practical issues. Give overview to verification and validation of methods. Give insight into the particulate science research challenges for successful application of methods to industrially relevant problems in particle technology.

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

3.2	In Scope	Quantum DFT, molecular dynamics, Finite Element Methods with multiple free and moving boundaries and multi-physics, Solid Mechanics, Lattice Boltzmann, CFD, Population Balance, Volume of Fluid Methods, Phase Field, Kinetic Monte Carlo, particle-CFD coupling, Stokesian Dynamics, Brownian Dynamics, etc.
	Out of Scope	DEM
4.0	Contractor(s) with contact information	Sundaresan (Princeton),
4.1	Comments / experiences	



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Synthesis of Particle Processing Systems
1.1	Project / Review	Roundtable
1.2	Technical Area	Systems
2.0	Submitted by	B. Diemer, S. Bermingham, J. Moser, M. Pasha, K. Keller, J. Lechman, E.Saurer
2.1	Member company/ies	PSE, Merck, Chemours, Sandia
2.2	Idea creation date	June 20, 2017
2.3	Last modification date	June 21, 2017
3.0	Short goal description	Develop a path toward codifying a hierarchical structure of decisions which must be made in creating integrated particle processes and a set of heuristics for use in making these decisions.
3.1	Objectives	Hold a roundtable in which: (a) members and invited guests share methodologies used for this purpose at their companies, or known procedures used for chemical process synthesis (such as the 5-step Douglas method), (b) a set of key issues needing resolution is developed (c) an course of action to achieve the goal is developed
3.2	Scope	Process steps to be considered should deal with particle formation and growth, particle separations, particle modification, and particle packaging (at a minimum) in as generic a sense as possible. The discussion will be at the conceptual level and not deal with design of individual unit ops but rather their sequencing as guided by product particle requirements.
4.0	Contractor	B. Diemer in conjunction with a Roundtable Development Team of 2-4 others drawn from the membership.
4.1	Comments / experiences	B. Diemer teaches the capstone chemical engineering design course at University of Delaware in which the Douglas 5-step hierarchical synthesis procedure (with heuristics) is used for the process synthesis aspect of design. He also teaches the product engineering course in the UD Master of Engineering in Particle Technology program, and has attempted to bolt-on some particle aspects to the Douglas method as well as including those few that Douglas employs. It is his assessment that this is not adequate for highly effective/efficient particle processing system synthesis.



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	(Working) Title	Real Time Measurement of Agglomerate Strength During Conveyance
1.1	Project or Review	Workshop
1.2	Technical Area ¹	Characterization
2.0	Submitted by	Rick Cook, Bill Schwerin
2.1	Member company/ies	Energizer, Honeywell-UOP
2.2	Idea creation date	6/20/2017
2.3	Last modification date	
3.0	Short goal description	Develop a macro-scale characterization methodologies for real-time analysis of defects & damage for process-control feedback.
3.1	Objectives	Identify real-time measurement techniques to detect defects and damage. Define constraints & limitations of existing technologies. Detail a roadmap for future improvements.
3.2	Scope	Dry flow, Powders
4.0	Contractor(s) with contact information	Mojtaba Ghadiri or Jim Litster
4.1	Comments / experiences	

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



IFPRI PROJECT / REVIEW BRIEF TEMPLATE

1.0	Working Title	Suspensions and slurries: insights from new physics
1.1	Project or Review	Workshop
1.2	Technical Area ¹	Wet Systems
2.0	Submitted by	Wilson Poon, Scott Brown, Marty Murtagh, Norman Wagner, John Hone
2.1	Member company/ies	
2.2	Idea creation date	20 June 2017
2.3	Last modification date	
3.0	Short goal description	Diverse processes in suspensions and slurries are of interest to IFPRI members: from incorporation and granulation through the effect of particle shape on extrusion to the aging of colloidal gels. Alongside particle technologists, soft matter physicists also work intensively on such topics. To date, there have been few organized attempts to bring these communities together. At the same time, significant new insights have been obtained by soft matter physicists, e.g. the role of particle contacts in controlling rheology, and therefore the potential of a unified description of dry granular flow and concentration suspension rheology, rigidity percolation in gel formation, or the origins of aging in colloidal gels . We therefore propose a workshop to enable such cross-fertilization between the two communities.
3.1	Objectives	To provide a forum for scientists and engineers working on fundamental aspects of wet particle systems to expound new advances from their perspective, and for particle technologists to explain the applications challenges. A round-table discussion to produce a road map for future directions to enable sustained, closer interaction between the two communities for both immediate scientific impact and for longer-term training and educational dividends.
3.2	Scope	Industrial processes and products that use or go through suspensions, slurries and pastes, and relevant, fundamental advances in soft matter physics, including experiment, theory and simulation.
4.0	Contractor(s) with	

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

	contact information	
4.1	Comments / experiences	This workshop is intended to follow on the gel workshops at Delaware and Crete, and as such, should provide a roadmap for wet systems. Holding this at the Edinburgh meeting is especially attractive given the strengths in soft matter physics and industrial applications of particle technology associated with this University and its faculty.