Workshop (Monday, 09 December, optional event limited to a small group)

Calibration and validation of numerical simulations: methods and challenges updated 01dec19

Hao Shi (MercuryLab B.V., University of Twente), Martin Bennett (Huxley Bertram, Cambridge UK), Stefan Luding (Multi Scale Mechanics, University of Twente)

The ever-increasing computer power offers the possibility to simulate complex processes numerically, using the Discrete Element Method (DEM) in virtually reproducing the discrete features of materials, such as granules and powders. This exacerbates the challenge of setting up simulations for different industrial applications. One popular approach to set up inputs in the discrete simulations is to use the particle properties measured experimentally at the microscale, e.g. particle density, stiffness and friction. This approach becomes extremely difficult when the particles are too small, sticky or exhibit irregular shapes. Another approach to address this challenge is "calibration", whereby the particle properties are derived as adjustable parameters by quantitative comparison of bulk properties and flow behaviour on the macroscale experimental and simulation results. The calibration approach often needs a validation after the parameters have been calibrated, in which the final set of calibrated parameters is validated using a second experiment. The validation might not work well if a mis-selection of the calibration experiments or the wrong solutions from multisolution space of the calibrated parameters are chosen.

This workshop is limited to 24 participants and will address cutting edge methods in calibration approaches and highlight some of the key issues and challenges presented by this Calibration & Validation methodology (C&V).

12:00 welcome and introduction (workshop registration starts at 11:15 in the lobby of the U Parkhotel, then proceed to meeting Room 1300, Horst Tower)

12:15 short presentations

Stefan Luding	University of Twente	terminology, approaches, challenges and recommendations
Jerome B. Johnson	Coupi Inc.	The importance of calibration, verification & validation in mechanistic modeling
Anthony Thornton	U. of Twente; MercuryLab B.V.	Bayesian calibration/validation & uncertainty propagation

13:30 Lunch break

14:00 case studies and Lab tour (divided in 2 groups)

case study	blending & segregation	lab-scale characterisation of powders; testing devices
	Anthony Thornton, Hao Shi	Effect of particle size and cohesion on powder yielding and flow (Hao Shi)
case study	powder compaction	double-ended compaction simulation of powders
	Martin Bennett, Luca Orefice	

16:30 reunion of the two groups and coffee break

16:45 partner presentations: Filip Francqui (Granutools), Michael Bradley (The Wolfson Centre), Johan Groen (Delft Solids Solutions)

17:45 discussion, recommendations and conclusion

18:15 end of workshop, proceed to the Welcome Reception at the hotel. **The Reception is sponsored by Rocky DEM**

Scientific Conference (Tuesday/Wednesday, 10-11 December)

Keynote speakers:

Michael Bradley Wolfson Centre, University of Greenwich (UK)	**An industrial overview of causes, effects, consequences, solutions and the current state of art in material characterisation and problem prediction**
J.M.N.T (Nico) Gray University of Manchester (UK)	**Particles segregation in dense granular flows**
Stefan Luding University of Twente (NL)	**Review on segregation in flowing and vibrated granular systems**
Benjy Marks University of Sydney (AU)	**Segregation, mixing and breakage during granular flow**
Paul Mort Purdue University, previously P&G (US)	**Powder flow and cohesion - balancing industrial and academic perspectives of product design and processing**
Anthony Thornton University of Twente (NL); MercuryLab B.V.	**Multiscale modelling of industrial granular materials**
Jan Wieringa Unilever (NL)	**An industrial view on blending and segregation of consumer goods**

In addition, the 2-day Scientific Conference will offer:

- **14 podium presentations (30 minutes each) by experienced practitioners and researchers**
  the current schedule of podium presentations can be viewed under the website's **CONFERENCE SCHEDULE** tab

- **four sessions:** overview of mixing/demixing aspects — current research
  modelling & simulation — experimental aspects, applications and case studies
- **industrial applications and case studies**

- **student events: flash presentations and posters display/competition (Tuesday)**
- **Social events: Welcome Reception (Monday at 18:00), Posters Reception and Forum Dinner (Tuesday)**

Symposium (Thursday, 12 December, optional event limited to a small group)

motivation

Rotary tablet presses have existed for about a century and evolved into ubiquitous, sophisticated pharmaceutical processors. Even though significant progress is being made, insufficient scientific basis exists to support their design/behaviour and much remains to be known about the attendant challenge of high-speed die compaction. Similarly, the punches and dies which form the tablets are critical, as they control the production performance of a press.

With the advent of pharmaceutical continuous tabletting, operational issues such as punch sticking, lamination/capping and feeding have come to the forefront and are to be addressed scientifically if the rotary tablet press unit operation is to become a truly-continuous process.

In parallel, material-sparing requirements and rational design approaches have increased the profile of press simulators and significant work is now being dedicated to the development of die compaction models which will lead us to the next level of the material-sparing paradigm.

This 6-hour intense symposium is limited to a small group and gathers presses/compaction experts who attended the Conference and are willing to update the group on their recent findings and research. Critical topics such as punch sticking, compaction models, feeders and PAT aspects will be explored.

8:45 introduction: scientific aspects of rotary tablet presses: design/operation, PAT and die compaction

9:00 casual presentations/discussions focused on rotary tablet presses, including modeling and simulation of die compaction (limited to a small group)

- Anton Kulchitsky & Jerome B. Johnson — Coupi, Inc
- Anthony Thornton & Thomas Weinhart — MercuryLab
- Theresa Hoermann & Luca Orefice — RCPE, Graz
- Paul Mort — Purdue University, previously P&G
- Martin Bennett — Huxley Bertram
- Robert Sedlock — Natoli

11:00 presentation and discussion of die compaction numerical models:

- the modelling challenges of die compaction
- MercuryLab B.V.
- University of Twente
- Coupi Inc.
- RCPE, Graz

13:30 short presentations (continued)
the following topics will be presented during the morning & afternoon discussions:

- the discrete nature of punch sticking and how to characterise it
- the effects of production press stiffness on tablet compaction strain rate
- simulation of load-limiting presses using a compaction simulator
- powder handling/feeding and mechanical aspects of rotary tablet presses
- suitability of existing rotary press feeders for continuous tableting

15:00 conclusion of the Symposium and end of Forum

Tuesday 10 December: Scientific Conference, day 1

01dec19

8:00	**Registration & Introduction**		**Session 1: overview of mixing/demixing (solid-solid systems)**
8:30	**Stefan Luding**	University of Twente	Review on segregation in flowing and vibrated granular systems
9:15	**Jan Wieringa**	Unilever	An industrial view on blending and segregation of consumer goods
10:00	**morning break (15 minutes)**		
10:15	**Mike Bradley**	The Wolfson Centre for bulk solids handling technology	An industrial overview of causes, effects, consequences, solutions and the current state of art in material characterisation and problem prediction
11:00	Barbara Schönfeld	AbbVie Germany	In-line blend uniformity monitoring using near-infrared spectroscopy as PAT tool
11:30	Wouter K. den Otter	University of Twente	Segregation of granular particles by mass, radius and density in a horizontal rotating drum
12:00	Bastiaan HJ Dickhoff	DFE pharma	How to approach mixing for challenging low dose pharmaceutical formulations and how can continuous mixing play a role?
12:30	**Lunch break (60 minutes)**		**Session 2: current research**
13:30	**Benjy Marks**	University of Sydney	segregation, mixing and breakage during granular flow
14:15	Susantha Dissanayake	The Wolfson Centre for bulk solids handling technology	Cellular automata modelling for simulating segregation of wood pellets in silo filling and discharge
14:45	Kasper van der Vaart	University of Twente	Granular buoyancy in the context of segregation of single large grains in dense granular flows
15:15	**afternoon break (15 minutes)**		
15:30	Theresa Hörmann	RCPE, Graz	Production of tablets at RCPE's continuous wet granulation tableting line

16:00 flash presentations, followed by posters presentation and reception, **sponsored by GRANUTOOLS**

19:30 Forum dinner

notes:
1-keynote presentations are highlighted in blue
2-Conference content and speakers placement are preliminary; final content/placement will be available one week before the Forum
3-to view the Wednesday programme (second day of the Scientific Conference), move your pointer over the bottom of this page

Wednesday, 11 December: Scientific Conference, day 2

8:00	**Introduction**		**Session 3: Modelling & Simulation**
8:15	**Nico Gray**	University of Manchester	Particle segregation in dense granular flows
9:00	**Anthony Thornton**	U. of Twente; MercuryLab	Multiscale modelling of industrial granular materials
9:45	**morning break** (30 minutes)		
10:15	Anton Kulchitsky	Coupi, Inc.	IBC blending performance analysis depending on particle dimension & shape
10:45	Thomas Weinhart	Twente/MercuryLab B.V.	Coarse-graining with MercuryCG - from discrete particles to continuum fields
11:15	Marina Sousani	DEM Solutions Ltd	Understanding the mechanistic behaviour of powder mixing with the use of DEM modelling & simulation
11:45	Clovis Maliska, Jr.	ESSS Ltd, Brazil	Next-generation DEM technology using Rocky: some examples and case studies of blending, mixing and segregation in practical applications
12:15	**Lunch break** (75 minutes)		**Session 4: experimental aspects, case studies & applications**
13:30	**Paul Mort**	Purdue University (ex P&G)	Powder flow and cohesion - balancing industrial and academic perspectives of product design and processing
14:15	Patrick Verolme	Delft Solids Solutions	Determining the amount of segregation using analytical measurement methods
14:45	Mike Bradley	The Wolfson Centre for bulk solids handling technology	Influences of flowability and permeability on air elutriation segregation of pharmaceutical powders
15:15	**afternoon break** (15 minutes)		
15:30	Naveen Mani Tripathi	Granutools	Physical characterization of powder blends with a focus on electrostatic properties
16:00	Olukayode Imole	Hosokawa Micron B.V.	Effect of process variables and material flow on filling consistency and final performance of lactose-based dry powder inhaler formulations
16:30	discussion & conclusion		
17:30	**End of the BSF2019-EU Scientific Conference**		