

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

Calibration and validation of numerical simulations: methods and challenges updated 21nov19

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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 Park Hotel)

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	MercuryLab B.V.	Bayesian calibration/validation & uncertainty propagation

13:30 Lunch break

14:00 case studies (divided in 2 groups)

case study	mixing & segregation	lab-scale characterisation of powders; testing devices
case study	powder compaction	Effect of particle size and cohesion on powder yielding and flow (Hao Shi) double-ended compaction simulation of powders

16:30 reunion of the two groups and coffee break

16:45 partner presentations

17:45 discussion, recommendations and conclusion

18:30 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)

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 tableting, 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)

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| • 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.
- 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

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8:00 Registration & Introduction

8:30 **Stefan Luding** University of Twente

9:15 **Jan Wieringa** Unilever

10:00 morning break (15 minutes)

10:15 **Mike Bradley** The Wolfson Centre
for bulk solids handling technology

11:00 Barbara Schoenfeld AbbVie Germany

11:30 Wouter K. den Otter University of Twente

12:00 Bastiaan HJ Dickhoff DFE pharma

Session 1: overview of mixing/demixing (solid-solid systems)

Review on segregation in flowing and vibrated granular systems

An industrial view on blending and segregation of consumer goods

An industrial overview of causes, effects, consequences, solutions
and the current state of art in material characterisation and problem prediction

In-line blend uniformity monitoring using near-infrared spectroscopy as PAT tool

Segregation of granular particles by mass, radius and density in a horizontal rotating drum

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

14:15 Susantha Dissanayake The Wolfson Centre
for bulk solids handling technology

14:45 Kasper van der Vaart University of Twente

segregation, mixing and breakage during granular flow

Cellular automata modelling for simulating segregation of wood pellets
in silo filling and discharge

Granular buoyancy in the context of segregation of single large grains in
dense granular flows

15:15 afternoon break (15 minutes)

15:30 Theresa Hoermann 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

8:15 **Nico Gray** University of Manchester
9:00 **Anthony Thornton** MercuryLab B.V.

Session 3: Modelling & Simulation

Particle segregation in dense granular flows
Multiscale modelling of industrial granular materials

9:45 morning break (30 minutes)

10:15 Anton Kulchitsky Coupi, Inc.
10:45 Thomas Weinhart MercuryLab B.V.
11:15 Marina Sousani DEM Solutions Ltd
11:45 Clovis Maliska, Jr. ESSS Ltd, Brazil

IBC blending performance analysis depending on particle dimension & shape
Coarse-graining with MercuryCG - from discrete particles to continuum fields
Understanding the mechanistic behaviour of powder mixing with the use of DEM modelling & simulation
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)

13:30 **Paul Mort** Purdue University (ex P&G)
14:15 Patrick Verolme Delft Solids Solutions
14:45 Mike Bradley The Wolfson Centre
for bulk solids handling technology

Session 4: experimental aspects, case studies & applications

Powder flow and cohesion - balancing industrial and academic perspectives of product design and processing
Determining the amount of segregation using analytical measurement methods
Influences of flowability and permeability on air elutriation segregation of pharmaceutical powders

15:15 afternoon break (15 minutes)

15:30 Naveen Mani Tripathi Granutools
16:00 Olukayode Imole Hosokawa Micron B V.

Physical characterization of powder blends with a focus on electrostatic properties
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; [please register for the Thursday Symposium!](#)