

Workshop (Monday, 09 December, optional event)

Calibration and validation of numerical simulations: methods and challenges updated 26aug

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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).

10:30 Forum and workshop registration, welcome and introduction

11:15 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
Hongyang Cheng	MercuryLab B.V.	Bayesian calibration/validation & uncertainty propagation

12:45 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

15:45 reunion of the two groups

16:00 partner presentations

17:00 discussion, recommendations and conclusion

17:30 end of workshop, proceed to the Welcome Reception at the hotel (starting at 18:00)

Symposium (Thursday, 12 December, optional event)

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 processing at the end of the last century, operational issues such as punch sticking, lamination and capping 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
- Paul Mort Purdue University, previously P&G
- Martin Bennett Huxley Bertram

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

- the modelling challenges of die compaction
- MercuryLab B.V.
- Coupi Inc.

1:30 short presentations (continued)

the following topics will be presented during the morning & afternoon discussions:

- using PAT in a tablet press feed frame to support process understanding
- the effects of production press stiffness on tablet compaction strain rate
- simulation of load-limiting presses using a compaction simulator
- the discrete nature of punch sticking and how to characterise it
- powder handling/feeding and mechanical aspects of rotary tablet presses

3:00 conclusion of the Symposium and end of Forum